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A Model for Reaction Rates in Turbulent Reacting Flows

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SUMMARY

To account for the turbulent temperature and species-concentration fluctuations, a model is presented on the effects of chemical reaction rates in computer analyses of turbulent reacting flows. The analysis results in two parameters, called the temperature and species amplification ratios, which multiply the terms in the equations to describe the rates of production or depletion of the species (i.e., the reaction-rate equations). The amplification ratios are dependent upon the mean values and the intensity of the turbulent fluctuations of the temperature and species concentrations. Graphs are presented of the amplification ratios which will permit use of the model in existing turbulent flow-field analyses.

The model was used in a two-dimensional parabolic-flow computer code to compare the results obtained with experimental data available for an axisymmetric, supersonic-combustion, hydrogen jet burning in air. The theoretical results show some improvement in agreement with the experiment in the far field (i.e., greater than 20 jet diameters from the injection station) in the region near the jet centerline. Recommendations for further improvement of the model include additional assessment of several of the parameters which arise in the formulation of the model by additional comparisons with experimental data.

INTRODUCTION

The highly nonlinear coupling of turbulence and chemical reaction increases the difficulty involved in the numerical computation of turbulent reacting flows. This difficulty occurs when global models of the finite-rate reaction are employed, as well as with models incorporating detailed chemical kinetics (ref. 1). The necessity for dealing with detailed kinetics when modeling turbulent diffusion flames is made clear in reference 2. The problem dealt with herein is the modeling of turbulent reaction rates in the numerical computation of combustion flow fields which employ detailed chemical kinetic mechanisms. Most such analyses (e.g., ref. 2) employ the mean temperature to calculate the Arrhenius reaction-rate coefficient; the coefficient is then multiplied by mean values of the species concentrations to produce a pseudomean reaction rate. In the formulation developed herein, a turbulent mean reaction rate is proposed which involves terms which are the product of a mean rate coefficient and the mean of the product of the species fluctuations. Quantities termed "amplification ratios" (presented as a series of graphs), which are dependent upon the mean temperature, the mean species concentrations, and the intensity of the turbulent fluctuations of these quantities, multiply each pseudo reaction-rate term and effectively "correct" these terms to their turbulent mean values. The proposed model is applicable to global and quasi-global mechanisms (ref. 3), although the principal consideration here is the development of a computationally viable approach applicable to large chemical mechanisms.

Among the approaches previously employed is that used in reference 2 in which the unmixedness model suggested in reference 4 is applied to terms in the reaction-rate expressions which contain either the fuel or the oxidizer concentration. An alternative approach (refs. 5 to 7) solves transport equations for joint probability density functions (pdf) of the species using Monte Carlo solution methods. Other approaches which have been examined include the expansion of the exponential term in

the Arrhenius expression for the reaction-rate constant (ref. 8), and the asymptotic expansion approach in reference 9. Heuristic models (refs. 10 and 11) are designed to circumvent the requirement for detailed chemical kinetics entirely.

The model proposed herein is based upon the assumed pdf approach employed in a large number of prior studies (e.g., refs. 12 to 16). The particular approach suggested is described in the next section, where probability density functions for the temperature are examined. Also proposed in the next section is an assumed pdf model to deal with the turbulent fluctuations in the species concentrations. Results are presented using the proposed model to calculate a supersonic, axisymmetric flow field for which detailed experimental data were available.

The contributions of the following colleagues to the work reported herein are acknowledged: Paul J. Antaki, Eileen Foy, Deborah Goldstein, Gregory Kassar, and Gregory Ronan at The Cooper Union.

SYMBOLS

A	preexponential constant in rate coefficient equation
a_j	mass fraction of species j ($j = A_1, A_2, \dots$)
B	temperature exponent in rate coefficient equation
c_j	molar concentration of species j
d	diameter, m
E	activation energy, kJ-mole^{-1}
K_1, K_2, K_3, K_4	constants
k_b	backward reaction-rate coefficient
k_f	forward reaction-rate coefficient
$k(x)$	reaction-rate coefficient of fluctuating variable x
p	static pressure, Pa
pdf	probability density function
p_t	pitot pressure, Pa
$p(x)$	pdf of fluctuating variable x
q	a priori probability in joint most-likely pdf
R	gas constant

r	radius measured from jet centerline, m
r_j	dimensionless molar concentration of species j
T	temperature, K
T_A	ratio of activation energy to gas constant, K
t	dimensionless temperature
\dot{w}_j	instantaneous net rate of reaction of species j , moles-(m) ⁻³ s ⁻¹
$\bar{\dot{w}}_j$	time-averaged reaction rate of species j , moles-(m) ⁻³ s ⁻¹
$\dot{\bar{w}}_j$	pseudomean reaction rate of species j , moles-(m) ⁻³ s ⁻¹
x	distance along flow direction, m
Z_r	species amplification ratio
Z_t	temperature amplification ratio
$Z(x)$	amplification ratio of fluctuating variable x
λ	coefficient in most-likely pdf
ρ^*	correlation coefficient

Subscripts:

max	maximum
min	minimum
n	nozzle
ref	reference

Chemical notation:

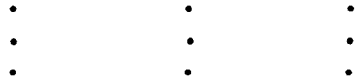
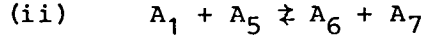
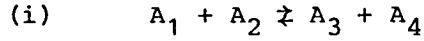
H ₂	hydrogen
H ₂ O	water
N ₂	nitrogen
O ₂	oxygen

A prime with a symbol denotes a fluctuating component.

DESCRIPTION OF REACTION-RATE MODEL

Assumed Probability-Density-Function Approach

For the general chemical kinetic mechanism



the instantaneous reaction rate of species A_1 is

$$\dot{w}_{A_1} = -k_{f,i} c_{A_1} c_{A_2} + k_{b,i} c_{A_3} c_{A_4} - k_{f,ii} c_{A_1} c_{A_5} + k_{b,ii} c_{A_6} c_{A_7} + \dots \quad (1)$$

where c_j is the molar concentration of species j .

In a turbulent flow, the turbulent mean value of \dot{w}_{A_1} is

$$\bar{\dot{w}}_{A_1} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} \dot{w}_{A_1} p(k_{f,i}, k_{b,i}, \dots, c_{A_1}, c_{A_2}, \dots) dT dc_{A_1} \dots$$

where $p(k_{f,i}, \dots)$ is the joint pdf of the indicated variables. Such a formulation cannot be modeled at present and is, in any event, mathematically intractable. Hence, it is proposed to treat each term in equation (1) separately and then sum, as follows:

$$\bar{\dot{w}}_{A_1} = \bar{\dot{w}}_{A_{1,1}} + \bar{\dot{w}}_{A_{1,2}} + \dots$$

where $\dot{w}_{A_{1,1}} = -k_{f,i} c_{A_1} c_{A_2}$, $\dot{w}_{A_{1,2}} = k_{b,i} c_{A_3} c_{A_4}$, etc., and where, for example,

$$\begin{aligned} \bar{\dot{w}}_{A_{1,1}} &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \dot{w}_{A_{1,1}}(k_{f,i}, c_{A_1}, c_{A_2}) p(k_{f,i}, c_{A_1}, c_{A_2}) dT dc_{A_1} dc_{A_2} \\ &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} k_{f,i} c_{A_1} c_{A_2} p(k_{f,i}, c_{A_1}, c_{A_2}) dT dc_{A_1} dc_{A_2} \end{aligned} \quad (2)$$

If it is further assumed that the turbulent temperature fluctuations are statistically independent of the fluctuations of the species concentrations (they are, of

course, mutually dependent through the transport equations describing the turbulent flow field), then equation (2) may be written

$$\bar{w}_{A_1,1} = \left[\int_{-\infty}^{\infty} k_{f,i}(T) p(T) dT \right] \left[\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} c_{A_1} c_{A_2} p(c_{A_1}, c_{A_2}) dc_{A_1} dc_{A_2} \right] \quad (3)$$

where $p(T)$ is the pdf of the temperature and $p(c_{A_1}, c_{A_2})$ is the joint pdf of the species concentrations. Although this assumption of statistical independence cannot be justified a priori on physical grounds, it is demonstrated later in this section that the results produced by a fully dependent statistical model do not differ greatly from the model proposed here. On the other hand, the proposed model is, from a computational standpoint, substantially simpler to incorporate into existing computer programs.

The integrals in equation (3) may be bounded between zero and unity by the introduction of the following parameters: The dimensionless temperature

$$t = \frac{T - T_{\min}}{T_{\max} - T_{\min}} \quad (4)$$

and the dimensionless molar concentration of species j

$$r_j = \frac{c_j - c_{j,\min}}{c_{j,\max} - c_{j,\min}} \quad (5)$$

where the quantities T_{\min} , T_{\max} , $c_{j,\min}$, and $c_{j,\max}$ represent appropriate minimum and maximum values of the variables, specified a priori. For example, T_{\min} could be the initial reactant temperature and T_{\max} the adiabatic flame temperature. Also $c_{j,\min}$ is zero and $c_{j,\max}$ would be the initial value for a reactant species, the final equilibrium value for a product species, or an estimated maximum for an intermediate species.

Since

$$k(T) = AT^B \exp(-T_A/T) \quad (6)$$

the first bracketed term on the right side of equation (3) can be rewritten

$$\int_{-\infty}^{\infty} k_{f,i}(T) p(T) dT = \int_0^1 \left[A(K_1 t + K_2)^B \exp\left(\frac{-T_A}{K_1 t + K_2}\right) \right] p(t) dt = \bar{k}(t) \quad (7)$$

where $K_1 = T_{\max} - T_{\min}$ and $K_2 = T_{\min}$. In similar fashion, the second bracketed term on the right side of equation (3) can be written

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} c_{A_1} c_{A_2} p(c_{A_1}, c_{A_2}) dc_{A_1} dc_{A_2} = \int_0^1 \int_0^1 (K_{3,A_1} r_{A_1} + K_{4,A_1}) \times (K_{3,A_2} r_{A_2} + K_{4,A_2}) p(r_{A_1}, r_{A_2}) dr_{A_1} dr_{A_2} \quad (8)$$

where $K_{3,j} = c_{j,\max} - c_{j,\min}$ and $K_{4,j} = c_{j,\min}$.

For computational purposes it is useful to rewrite the above relationships in the form

$$\bar{w}_{A_1,1} = Z \bar{w}_{A_1,1} = (Z_t \bar{k}_{f,i}) Z_r \bar{c}_{A_1} \bar{c}_{A_2} \quad (9)$$

where Z_t , the temperature amplification ratio, is equation (7) divided by equation (6); Z_r , the species amplification ratio, is equation (8) divided by the product $\bar{c}_{A_1} \bar{c}_{A_2}$, where \bar{c}_j is the mean value for species j ; and $Z = Z_t Z_r$. Thus, Z_t represents the ratio of the turbulent mean value of the Arrhenius reaction-rate constant to its value calculated by inserting the mean temperature into equation (6), and Z_r is the ratio of the turbulent mean value of the product $c_{A_1} c_{A_2}$ to the product $\bar{c}_{A_1} \bar{c}_{A_2}$.

Utilizing this formulation requires the selection of an appropriate pdf for the temperature (eq. (7)) and for the joint pdf of the species concentrations (eq. (8)). The selection of the pdf is discussed in the following sections.

Alternative Probability Density Functions for Modeling the Effect of the Temperature Fluctuations

Three probability density functions for the temperature were discussed in reference 17. These were the clipped Gaussian (ref. 12), the beta (ref. 18), and the ramp (ref. 19). The ramp probability density function has been observed in some regions of turbulent shear flows wherein temperature histories exhibit ramp-like behavior upon which high-frequency Gaussian fluctuations are superimposed (ref. 19). The principal conclusions reached in reference 17 concerning these three probability density functions are:

1. For all values of \bar{t} and $\overline{t'^2}$, the temperature amplification ratio Z_t is greater than unity; that is, the effect of the turbulent temperature fluctuations is to increase the effective Arrhenius reaction-rate constant.

2. Values of Z_t obtained using the clipped Gaussian pdf are substantially the same as those obtained using the beta pdf. Differences between the values obtained

for Z_t develop principally at low and high values of the mean temperature \bar{t} , which occur in regions where little reaction is occurring and where the reactions are nearing completion, respectively. This generally close correspondence in the behavior of the temperature amplification ratio Z_t for the clipped Gaussian and beta pdf leads one to choose the beta pdf for practical calculations because of the relative ease with which the beta pdf can be employed in computer programs.

3. Values of Z_t are substantially higher for the ramp pdf over the entire range of mean temperature \bar{t} than they are for either the clipped Gaussian or beta pdf.

An evaluation of the nonreactive flow-field data presented in references 20 to 23, wherein ramp-like behavior of the temperature fluctuations was observed in certain regions, leads to the following criterion for deciding whether to employ the beta pdf or the ramp pdf in equation (7) in a particular region of a turbulent flow field:

If $0.35 < \bar{t} < 0.75$ and $\overline{t'^2} > 0.08$, then the temperature fluctuations are likely to exhibit ramp-like behavior. Elsewhere, the beta pdf should be used in equation (7).

Another probability density function, not included in reference 17, is the "most-likely" pdf (ref. 5). Although it is computationally more difficult to utilize than the beta pdf, joint (multivariable) forms of the most-likely pdf can be written. As pointed out in reference 18, a physical basis exists for the use of the beta pdf to describe the turbulent fluctuations of many flow-field quantities. Hence, it was reasoned that if an essential equivalence could be demonstrated between the beta pdf and the most-likely pdf in its one-variable form, this would suggest the use of a bivariate form of the most-likely pdf to describe the species fluctuations.

The most-likely pdf (ref. 5), in its one-variable form, is given by

$$p(t) = \exp(\lambda_0 + \lambda_1 t + \lambda_2 t^2) \quad (10)$$

where the constant coefficients λ_0 , λ_1 , and λ_2 are obtained from simultaneous solution of the following constraint equations:

$$\int_0^1 p(t) dt = 1$$

$$\int_0^1 t p(t) dt = \bar{t}$$

$$\int_0^1 (t - \bar{t})^2 p(t) dt = \overline{t'^2}$$

Results obtained for Z_t using equation (10) in equation (7) are shown in figures 1 to 3. Parameter values for the cases cited in figures 1 to 3 are in table I. The most-likely pdf is compared with the beta pdf in the figures. The two

pdf's yield quite similar results over the examined ranges of \bar{t} and $\overline{t'^2}$, and both exhibited similar sensitivities to the activation energy and temperature exponent. Again, this similarity favors the computationally simpler beta pdf in large-scale computer programs. However, as described above, the essential equivalence between the beta and most-likely pdf has important implications in selecting an appropriate joint pdf for the species concentrations in equation (8). This equivalence is examined in the next section.

Two-Variable Probability Density Function for Modeling the Effect of the Species-Concentration Fluctuations

As noted in the preceding section, the similarity in the results obtained for the temperature amplification ratio Z_t using the experimentally verified beta pdf and the most-likely pdf suggests that a bivariate (or joint) form of the most-likely pdf serves to model the effects of the species-concentration fluctuations. To obtain values for the species amplification ratio Z_r in equation (9), the following bivariate most-likely pdf is used in equation (8):

$$p(r_{A_1}, r_{A_2}) = q \exp(\lambda_0 + \lambda_1 r_{A_1} + \lambda_2 r_{A_2} + \lambda_3 r_{A_1} r_{A_2}) \quad (11)$$

where the value of q , called an a priori probability in reference 5, was, in accordance with reference 5, set equal to unity. The values of the constant coefficients λ_0 , λ_1 , λ_2 , and λ_3 in equation (11) are obtained from the simultaneous solution of the following constraint equations:

$$\int_0^1 \int_0^1 p(r_{A_1}, r_{A_2}) dr_{A_1} dr_{A_2} = 1$$

$$\int_0^1 \int_0^1 r_{A_1} p(r_{A_1}, r_{A_2}) dr_{A_1} dr_{A_2} = \bar{r}_{A_1}$$

$$\int_0^1 \int_0^1 r_{A_2} p(r_{A_1}, r_{A_2}) dr_{A_1} dr_{A_2} = \bar{r}_{A_2}$$

$$\int_0^1 \int_0^1 (r_{A_1} - \bar{r}_{A_1})(r_{A_2} - \bar{r}_{A_2}) p(r_{A_1}, r_{A_2}) dr_{A_1} dr_{A_2} = \overline{r'_{A_1} r'_{A_2}}$$

The dimensionless mean species concentrations \bar{r}_{A_1} and \bar{r}_{A_2} are, as with

\bar{t} and $\overline{t'^2}$, quantities which are calculated from transport equations describing the turbulent flow field. The covariance $\overline{r'_{A_1} r'_{A_2}}$ is determined from

$$\overline{r'_{A_1} r'_{A_2}} = \rho^* \left(\overline{r'^2_{A_1} r'^2_{A_2}} \right)^{1/2} \quad (12)$$

where, as above, the dimensionless mean-square species-concentration fluctuations,

$\overline{r_{A_1}^{'2}}$ and $\overline{r_{A_2}^{'2}}$, are calculated using appropriate transport equations (e.g., ref. 2),

and where ρ^* is the correlation coefficient. The correlation coefficient ρ^* is a measure of the degree of linearity between r_{A_1} and r_{A_2} . Values of ρ^* near ± 1 reflect a high degree of linearity, and values near zero indicate a lack of linearity. Positive values of ρ^* indicate that as r_{A_2} increases, r_{A_1} increases; negative values of ρ^* indicate that as r_{A_2} increases, r_{A_1} decreases.

From the data in reference 24, values between -0.9 and -1.0 were determined for the correlation coefficient ρ^* between the temperature and the hydrogen concentration throughout the flow field. It was concluded that correlation coefficients of this magnitude appear to be realistic in at least some types of flows. Hence, for the present calculations, results were obtained for $\rho^* = \pm 0.9$.

Results for Z_r obtained using $\rho^* = -0.9$ over ranges of \bar{r}_{A_1} , \bar{r}_{A_2} , $\overline{r_{A_1}^{'2}}$, and $\overline{r_{A_2}^{'2}}$ are shown in figure 4. In all cases $Z_r < 1$. This implies that, in

general, for reaction-rate terms involving species whose concentrations are changing in opposite directions (one increasing and one decreasing, which leads to $\rho^* < 0$), the effect of the turbulent species fluctuations is to reduce the reaction rate. In the literature, this effect has often been referred to as unmixedness. This unmixedness effect is seen in figure 4 to predominate (low values of the species amplification ratio Z_r) when the mean concentrations of the species are low and turbulent fluctuations are large.

On the other hand, figure 5 (where $\rho^* = 0.9$) illustrates that for reaction-rate terms involving species whose concentrations are changing in the same direction (either both increasing or both decreasing, which leads to $\rho^* > 0$), the effect of the turbulent species fluctuations is to increase the reaction rate through an enhanced mixing effect. The effect is again greatest at low values of the mean species concentrations and at high values of the turbulent species fluctuations. These results suggest that these mixedness/unmixedness effects are likely to be greatest in the high-shear mixing regions of turbulent diffusion flames, where turbulent fluctuations are likely to be greatest.

In writing equation (3), statistical independence was assumed between the temperature fluctuations and the species fluctuations. To examine this assumption, the results presented herein were compared with the results obtained for an amplification ratio calculated assuming full statistical dependence between the temperature and species fluctuations. The results for this latter amplification ratio $Z(t, r_{A_1}, r_{A_2})$ were obtained by employing the following three-variable form of the most-likely pdf:

$$p(t, r_{A_1}, r_{A_2}) = q \exp\left(\lambda_0 + \lambda_1 t + \lambda_2 r_{A_1} + \lambda_3 r_{A_2} + \lambda_4 t r_{A_1} + \lambda_5 t r_{A_2} + \lambda_6 r_{A_1} r_{A_2}\right) \quad (13)$$

where, as in equation (11), q , the a priori probability, is set equal to unity. The values of $\lambda_0, \lambda_1, \dots, \lambda_6$ are obtained from known values of $\bar{t}, \bar{r}_{A_1}, \bar{r}_{A_2}, \overline{t'r'_{A_1}}, \overline{t'r'_{A_2}}$, and $\overline{r'_{A_1}r'_{A_2}}$ by employing the following constraint equations:

$$\int_0^1 \int_0^1 \int_0^1 p(t, r_{A_1}, r_{A_2}) dt dr_{A_1} dr_{A_2} = 1$$

$$\int_0^1 \int_0^1 \int_0^1 t p(t, r_{A_1}, r_{A_2}) dt dr_{A_1} dr_{A_2} = \bar{t}$$

$$\int_0^1 \int_0^1 \int_0^1 r_{A_1} p(t, r_{A_1}, r_{A_2}) dt dr_{A_1} dr_{A_2} = \bar{r}_{A_1}$$

$$\int_0^1 \int_0^1 \int_0^1 r_{A_2} p(t, r_{A_1}, r_{A_2}) dt dr_{A_1} dr_{A_2} = \bar{r}_{A_2}$$

$$\int_0^1 \int_0^1 \int_0^1 (t - \bar{t}) (r_{A_1} - \bar{r}_{A_1}) p(t, r_{A_1}, r_{A_2}) dt dr_{A_1} dr_{A_2} = \overline{t'r'_{A_1}}$$

$$\int_0^1 \int_0^1 \int_0^1 (t - \bar{t}) (r_{A_2} - \bar{r}_{A_2}) p(t, r_{A_1}, r_{A_2}) dt dr_{A_1} dr_{A_2} = \overline{t'r'_{A_2}}$$

$$\int_0^1 \int_0^1 \int_0^1 (r_{A_1} - \bar{r}_{A_1}) (r_{A_2} - \bar{r}_{A_2}) p(t, r_{A_1}, r_{A_2}) dt dr_{A_1} dr_{A_2} = \overline{r'_{A_1}r'_{A_2}}$$

A typical result is presented in figure 6, where $Z(t, r_{A_1}, r_{A_2})$ is the fully dependent amplification ratio calculated using equation (13), and $Z = Z_t Z_r$ is the result obtained assuming statistical independence between the temperature fluctuations and the species fluctuations. The results for this case are sufficiently similar in both magnitude and trend to support the assumption of statistical independence. In the next section, results are presented for a supersonic hydrogen-air diffusion flame for which experimental data were available.

APPLICATION OF THE MODEL TO A SUPERSONIC, AXISYMMETRIC FLOW

The chemical reaction model described in the previous sections was incorporated into the two-dimensional, parabolic computer program described in references 2

and 25. This program solves parabolic partial differential equations for the transport of the following quantities: mass, momentum, energy, species concentrations, turbulent kinetic energy, dissipation rate of turbulent kinetic energy, species concentration fluctuations, and temperature fluctuations. The program includes detailed chemical kinetics for describing chemical changes. The axisymmetric flow field examined (shown in fig. 7) consists of a supersonic hydrogen jet injected into a supersonic coaxial airstream. For these calculations, the eight-reaction H_2-O_2 chemical kinetic mechanism is shown in table II. The values of the forward reaction-rate constants are also in table II.

To utilize the portion of the model described herein dealing with the effect of the species-concentration fluctuations, a criterion is required for deciding whether to employ a positive or negative value for the correlation coefficient ρ^* . That is, at a particular location in the flow field one must decide whether the concentrations of the species involved in the reaction are mutually increasing or decreasing ($\rho^* = 0.9$) or whether one species is increasing in concentration while the other is decreasing ($\rho^* = -0.9$). To expedite the calculations, the point in the flow field (at a given axial location) where the hydrogen and oxygen were present in stoichiometric proportion was selected as the location for assigning particular trends to the species concentrations. For example, for radial values greater than that at the stoichiometric plane, water and the free radicals O, H, and OH were assumed to decrease in concentration as radius increased. Inside the stoichiometric location, these species were assumed to increase in concentration from the centerline to the stoichiometric point. On the other hand, H_2 was assumed to decrease monotonically and O_2 was assumed to increase monotonically from the centerline outward along the radius. As an example, for reaction 5 in table II, $\rho^* = 0.9$ in both the forward and backward directions. For reaction 8, H_2 and O were assumed to move in opposite directions from the centerline to the stoichiometric location ($\rho^* = -0.9$) and in the same direction ($\rho^* = 0.9$) outside the stoichiometric location. However, for reaction 8 proceeding from right to left, the correlation coefficient is always positive.

Results for the centerline hydrogen concentration calculated using instantaneous kinetics are compared with results obtained by incorporating the model proposed herein and with experimental values in figure 8. Slight improvement in the calculated values using the turbulence reaction model may be seen, particularly in the far field. Radial pitot-pressure profiles at several axial locations are shown in figure 9. Again, a slight improvement is brought about by the inclusion of the proposed model in the far field in the region between the centerline and the stoichiometric location. This improvement occurs as well for the radial species-concentration profiles shown in figure 10. Ramp-like temperature fluctuations were not encountered in any of the calculations described, because $\overline{t'^2}$ never exceeded 0.08.

The results obtained from the flow-field calculations presented suggest a number of model refinements which are recommended for further investigation. These refinements include the requirement for a more precise criterion to decide upon the sign of the correlation coefficient ρ^* . For example, rather than utilize the stoichiometric H_2-O_2 location as an arbitrary turnover point, the computer program could monitor the gradients of the species concentrations at previously calculated adjacent points to decide upon the sign of the correlation coefficient ρ^* . Ultimately, the magnitudes of the concentration gradients could be used to assign values to ρ^* between ± 1 , rather than using fixed values for ρ^* .

The criterion developed for observing ramp-like temperature fluctuations was based upon data obtained from nonreacting flows. Additional numerical experimentation based upon alternative criteria for introducing temperature-ramp values of the temperature amplification ratio Z_t needs to be undertaken so that recommendations can be made for reacting flows.

Additional calculations are required using chemical kinetic mechanisms other than the eight-reaction mechanism in table II. For example, reference 2 documents the improved correlation between calculated and experimental values obtained using a larger chemical mechanism for hydrogen-air combustion. The effects of the model presented here on a larger-scale chemical mechanism must be assessed.

CONCLUDING REMARKS

It has been shown that a computationally viable, three-variable (temperature and species concentrations) model for reacting flows which accounts for the effects of turbulence on chemical reaction rates results in some improvement in the agreement between the theoretical prediction and the data from an axisymmetric, supersonic-combustion, hydrogen-fueled experiment. The theoretical prediction of the flow parameters and species concentrations shows best agreement with the experiment in the far field (greater than 20 fuel jet diameters (x/d_{jet}) downstream of the point of injection). Recommendations are made for what are considered necessary improvements to the model. These include improvements in methods for selecting a correlation coefficient, alternative criteria for introducing temperature-ramp values of an amplification factor, and improved correlations by additional comparisons with experimental data.

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TABLE I.- TEST CASES

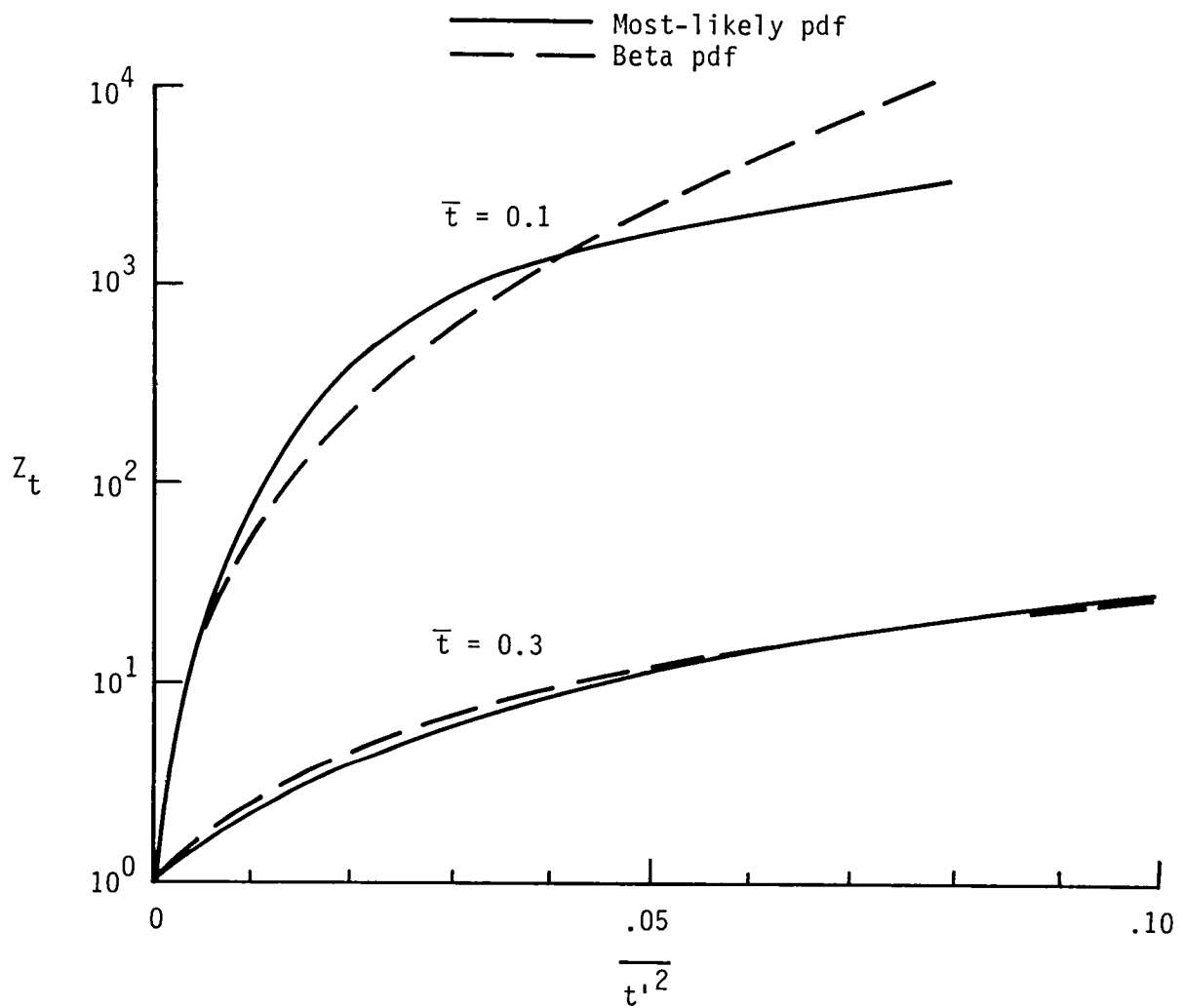
Case	A	B	T _A
1	8.4×10^{13}	0	10 116
2	8.4×10^{13}	0	5 000
3	8.4×10^{13}	1	10 116

Note: T_{min} = 500 K, T_{max} = 2500 K.

TABLE II.- CHEMICAL KINETIC MECHANISM AND RATE CONSTANTS

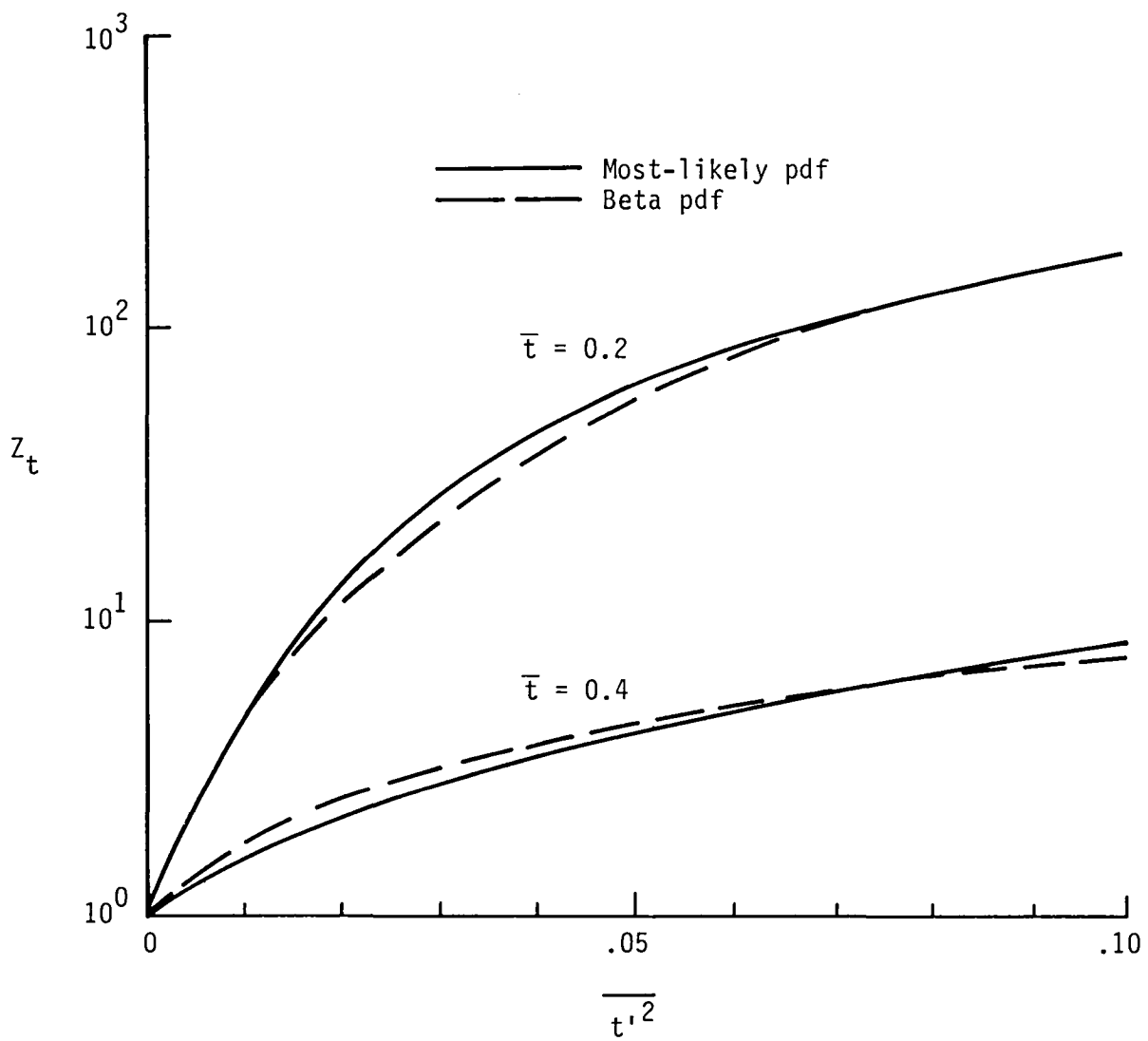
Reaction	Forward rate constant ^a		
	A	B	E
1. $\text{H}_2 + \text{M} \xrightarrow{k} \text{H} + \text{H} + \text{M}$	5.5×10^{18}	-1.0	51 087
2. $\text{O}_2 + \text{M} \xrightarrow{k} \text{O} + \text{O} + \text{M}$	7.2×10^{18}	-1.0	59 340
3. $\text{H}_2\text{O} + \text{M} \xrightarrow{k} \text{OH} + \text{H} + \text{M}$	5.2×10^{21}	-1.5	59 386
4. $\text{OH} + \text{M} \xrightarrow{k} \text{O} + \text{H} + \text{M}$	8.5×10^{18}	-1.0	50 830
5. $\text{H}_2\text{O} + \text{O} \xrightarrow{k} \text{OH} + \text{OH}$	5.8×10^{13}	0	9 059
6. $\text{H}_2\text{O} + \text{H} \xrightarrow{k} \text{OH} + \text{H}_2$	8.4×10^{13}	0	10 116
7. $\text{O}_2 + \text{H} \xrightarrow{k} \text{OH} + \text{O}$	2.2×10^{14}	0	8 455
8. $\text{H}_2 + \text{O} \xrightarrow{k} \text{OH} + \text{H}$	7.5×10^{13}	0	5 586

^aThe form of the rate constant is $k = AT^B \exp(-E/RT)$ with k in cm³/mole-s.



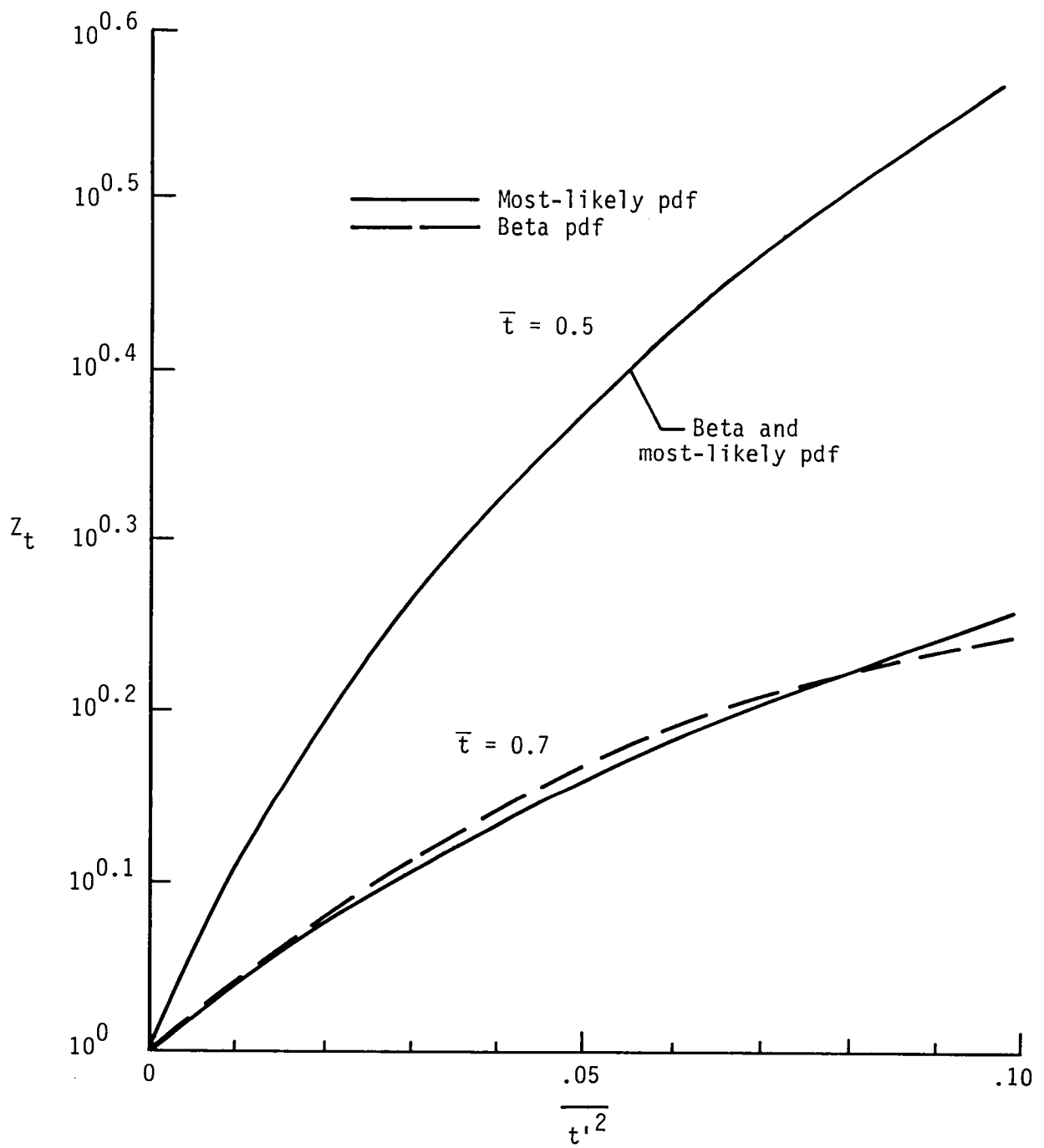
(a) $\bar{t} = 0.1$ and 0.3 .

Figure 1.- Comparison of results for beta pdf and most-likely pdf for case 1.



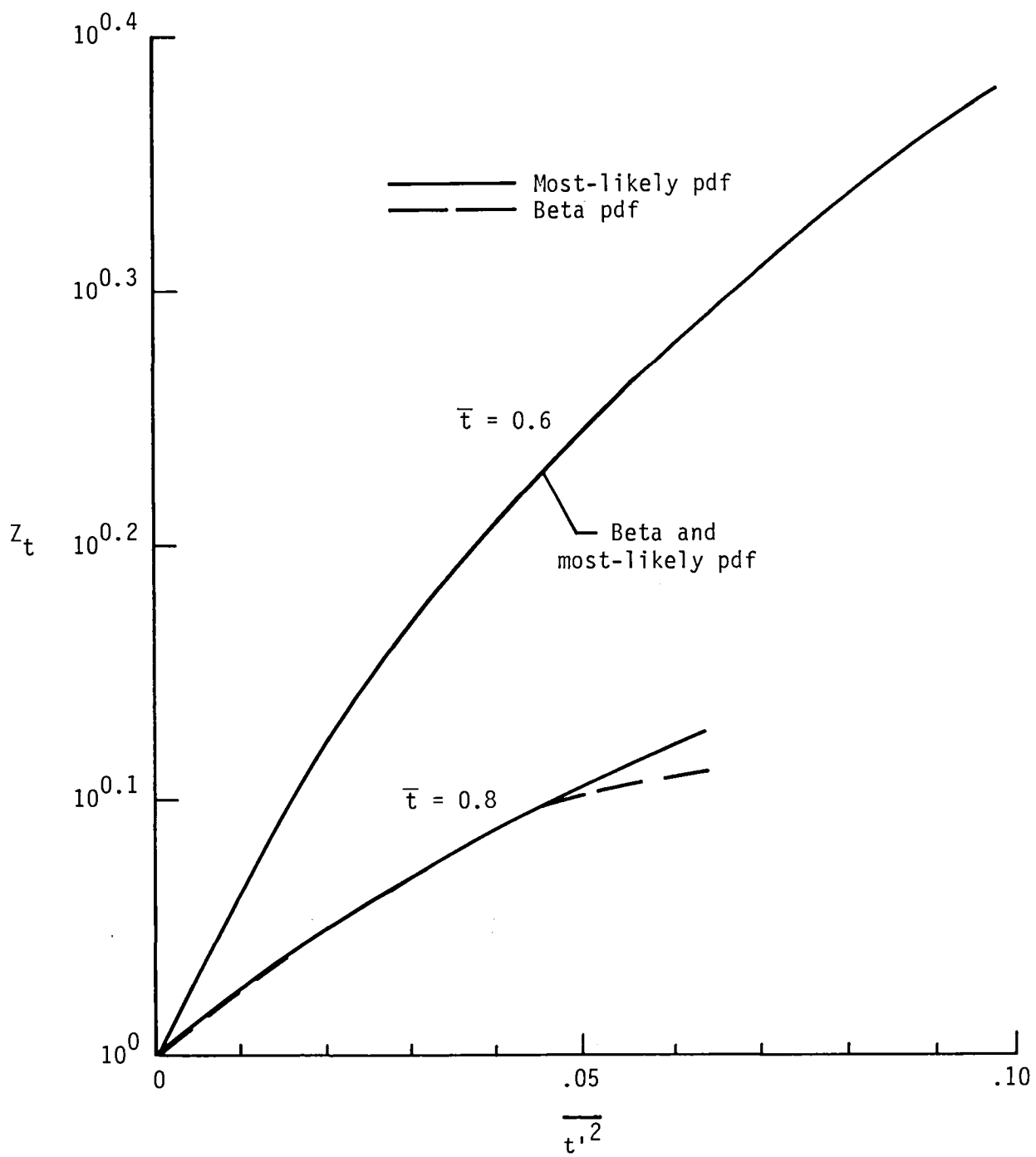
(b) $\bar{t} = 0.2$ and 0.4 .

Figure 1.- Continued.



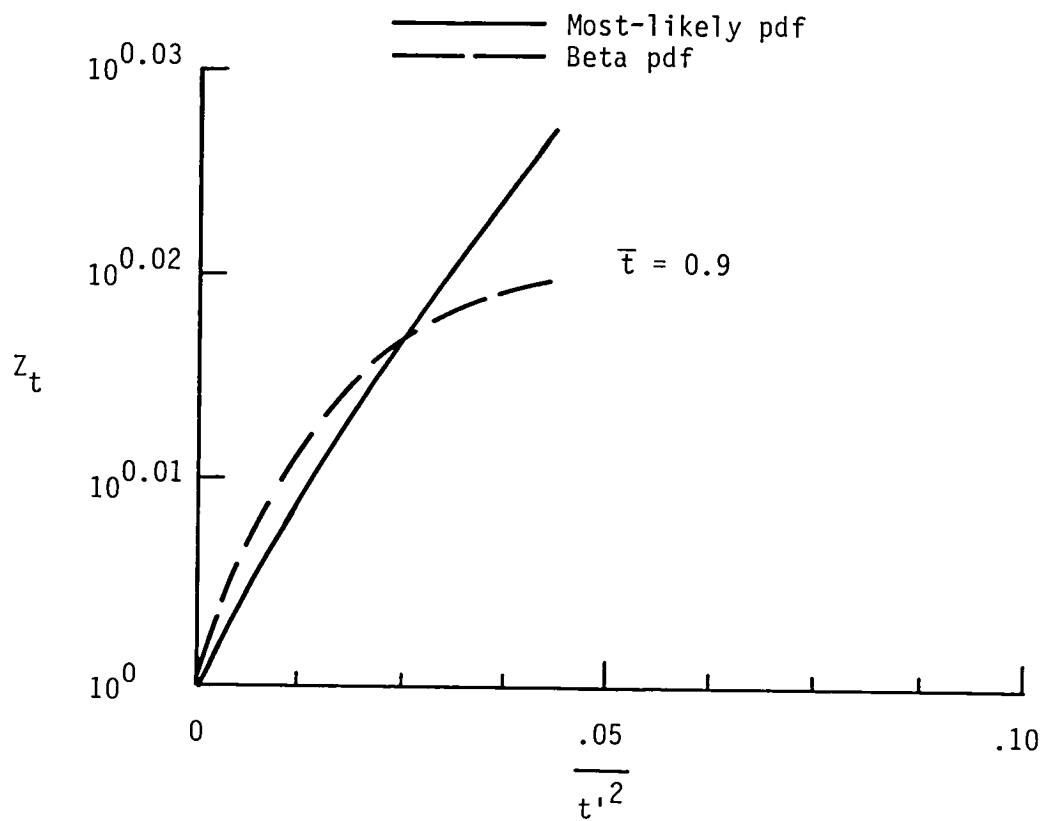
(c) $\bar{t} = 0.5$ and 0.7 .

Figure 1.- Continued.



(d) $\bar{t} = 0.6$ and 0.8 .

Figure 1.- Continued.



(e) $\bar{t} = 0.9$.

Figure 1.- Concluded.

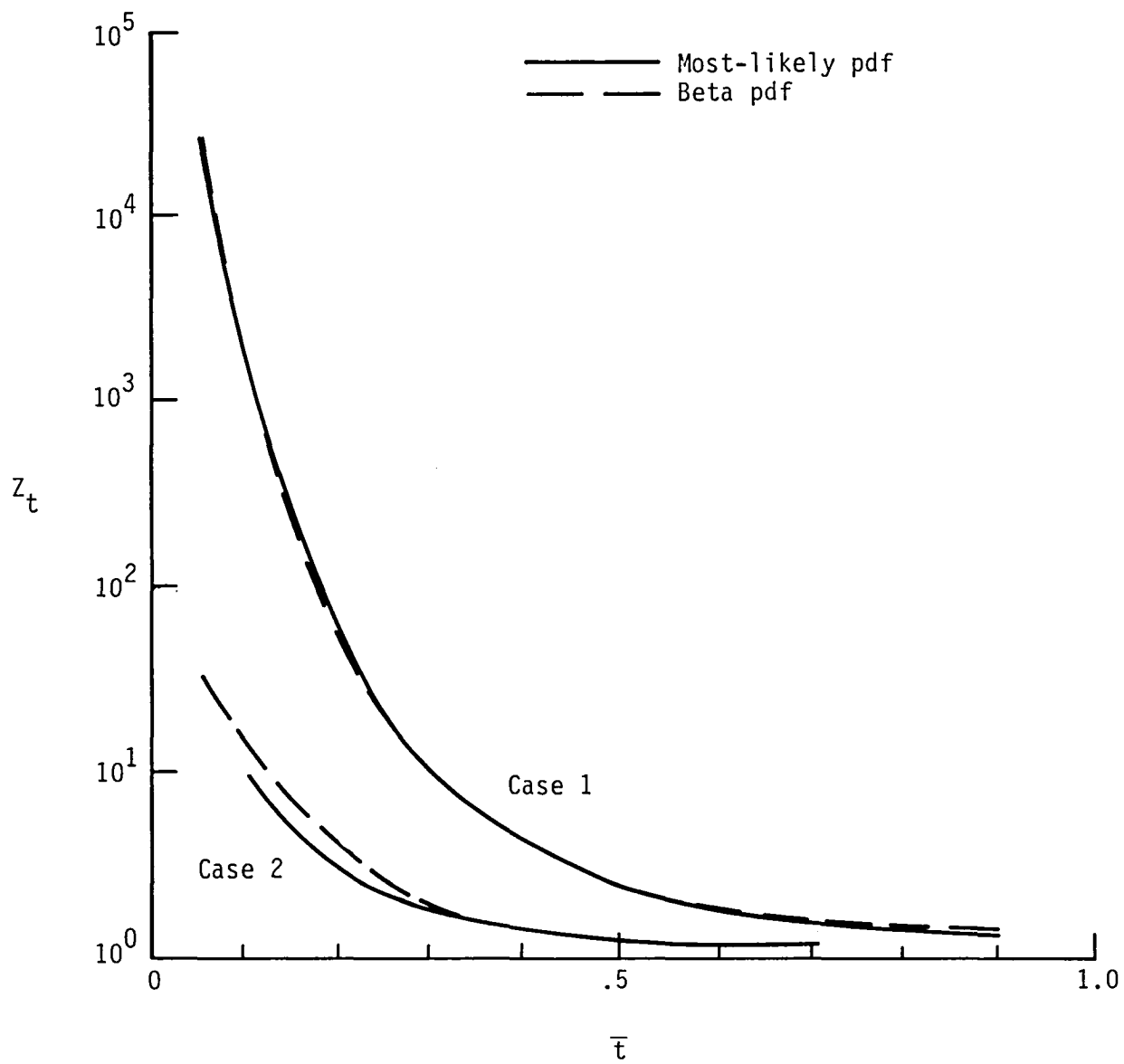


Figure 2.- Effect of activation energy on Z_t for beta pdf and most-likely pdf.
 $\overline{t'}^2 = 0.05$.

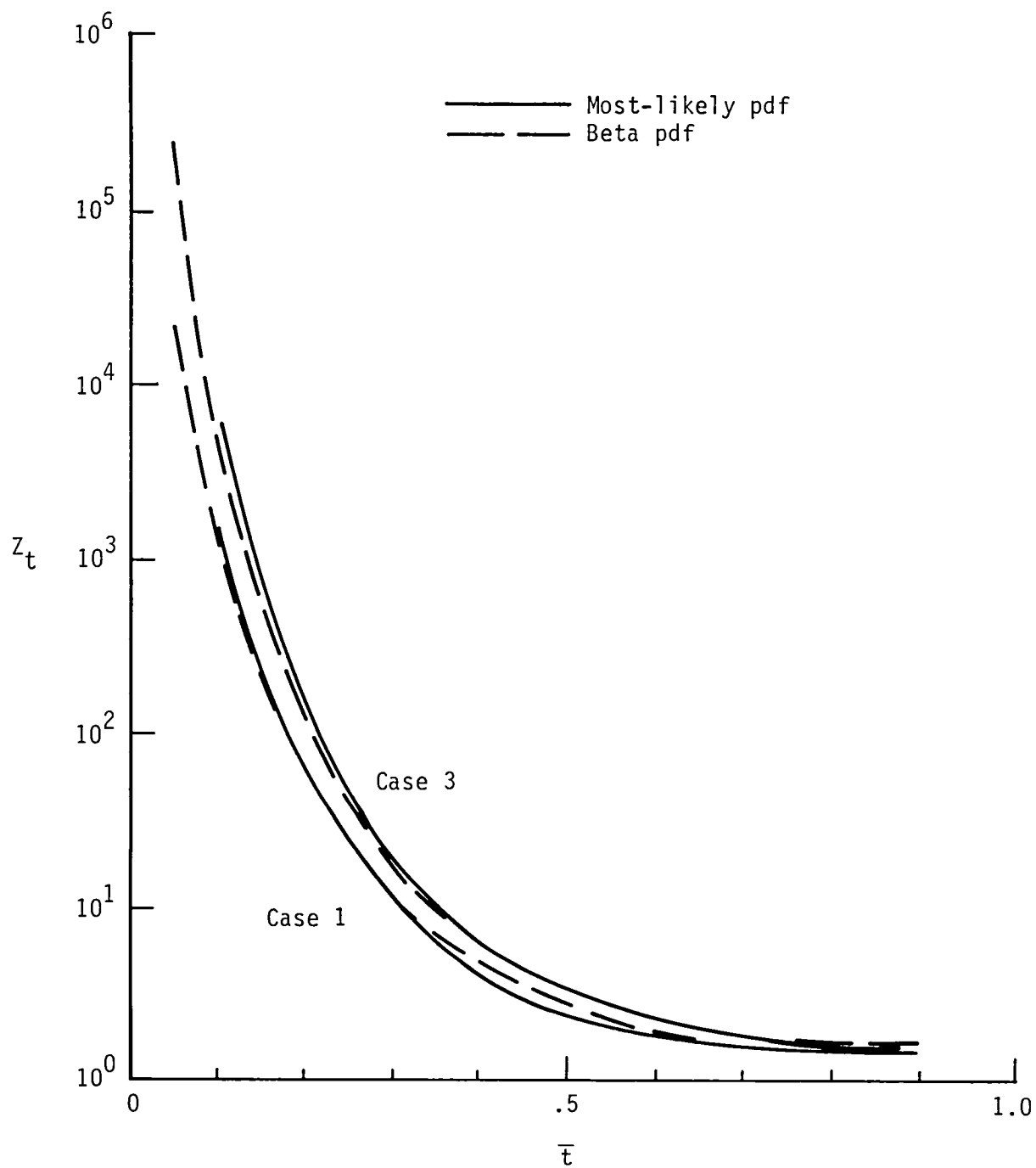
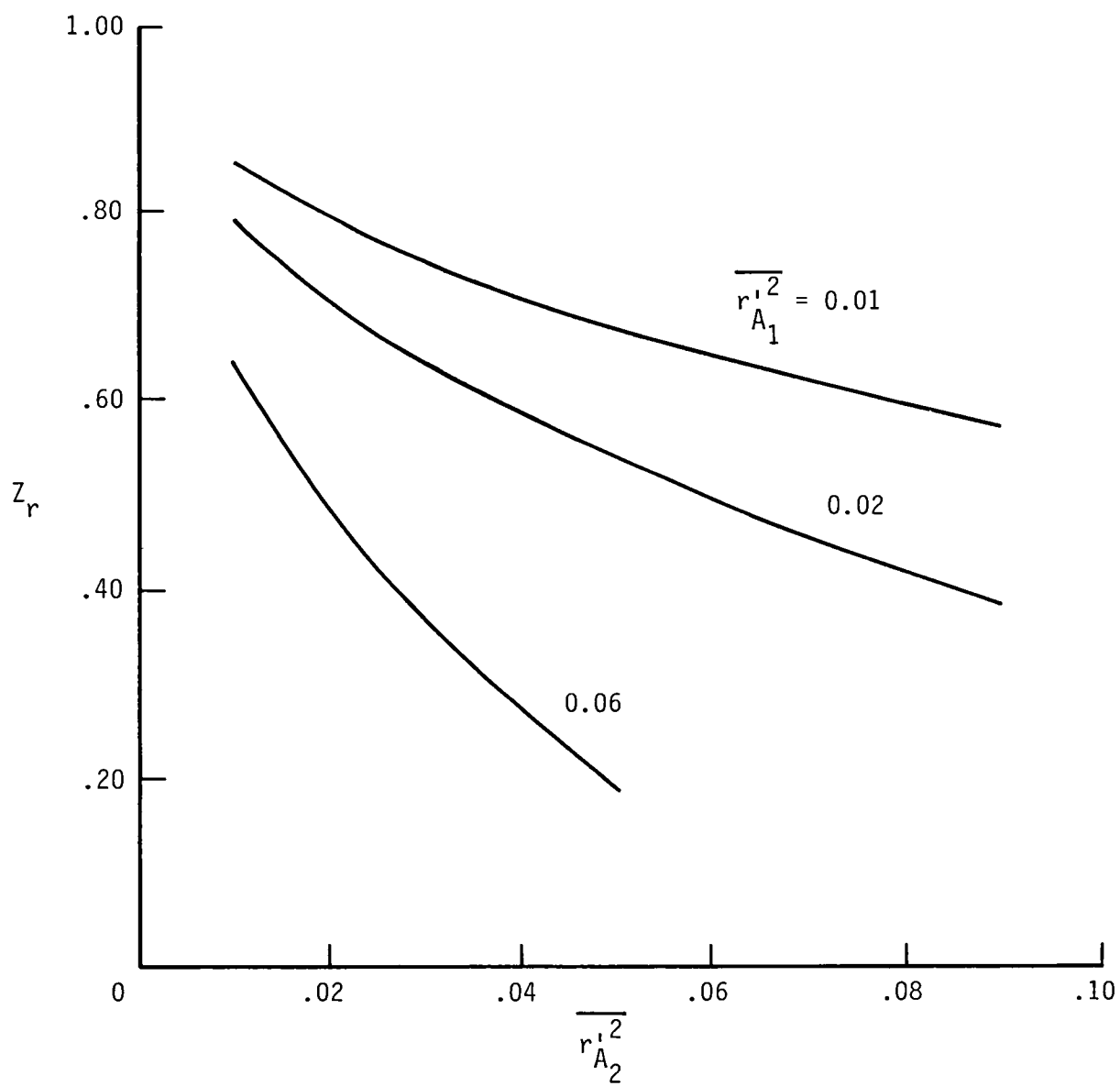
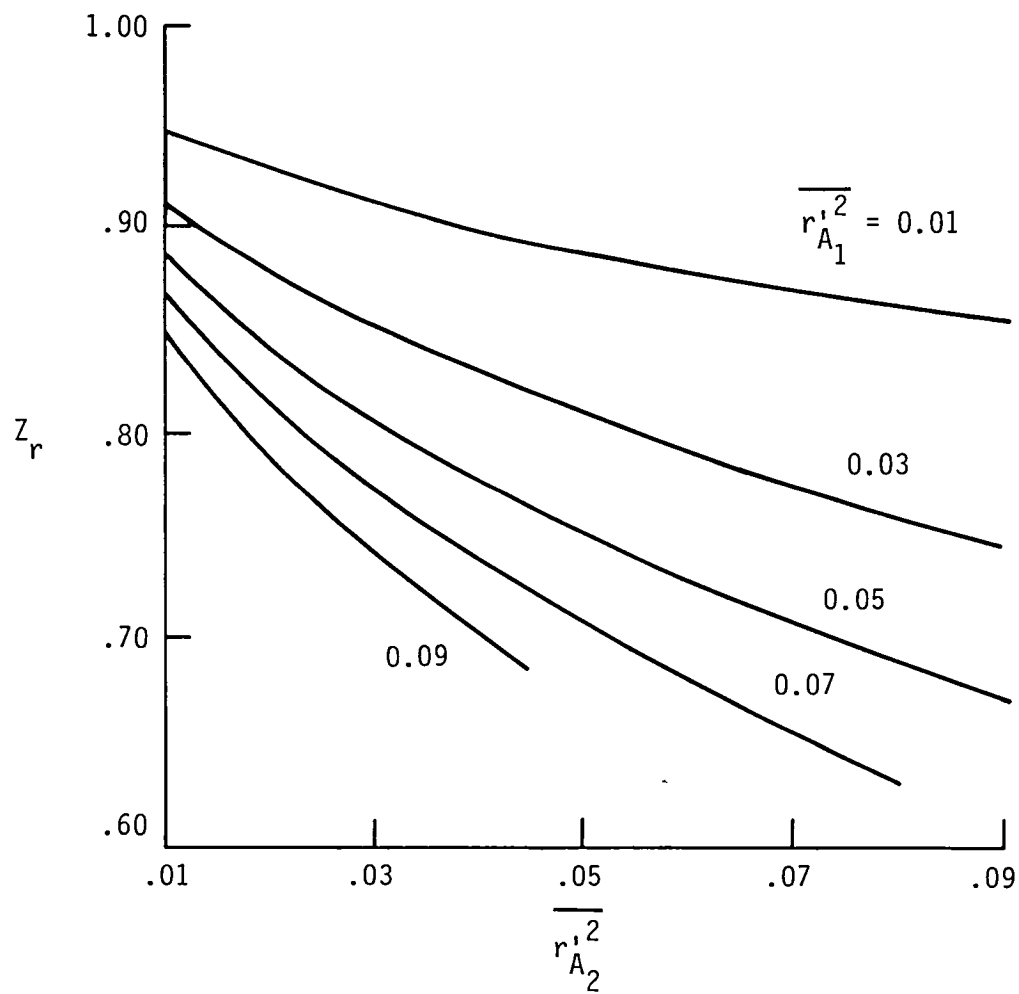


Figure 3.- Effect of temperature exponent on Z_t for beta pdf and most-likely pdf.
 $\overline{t'^2} = 0.05.$



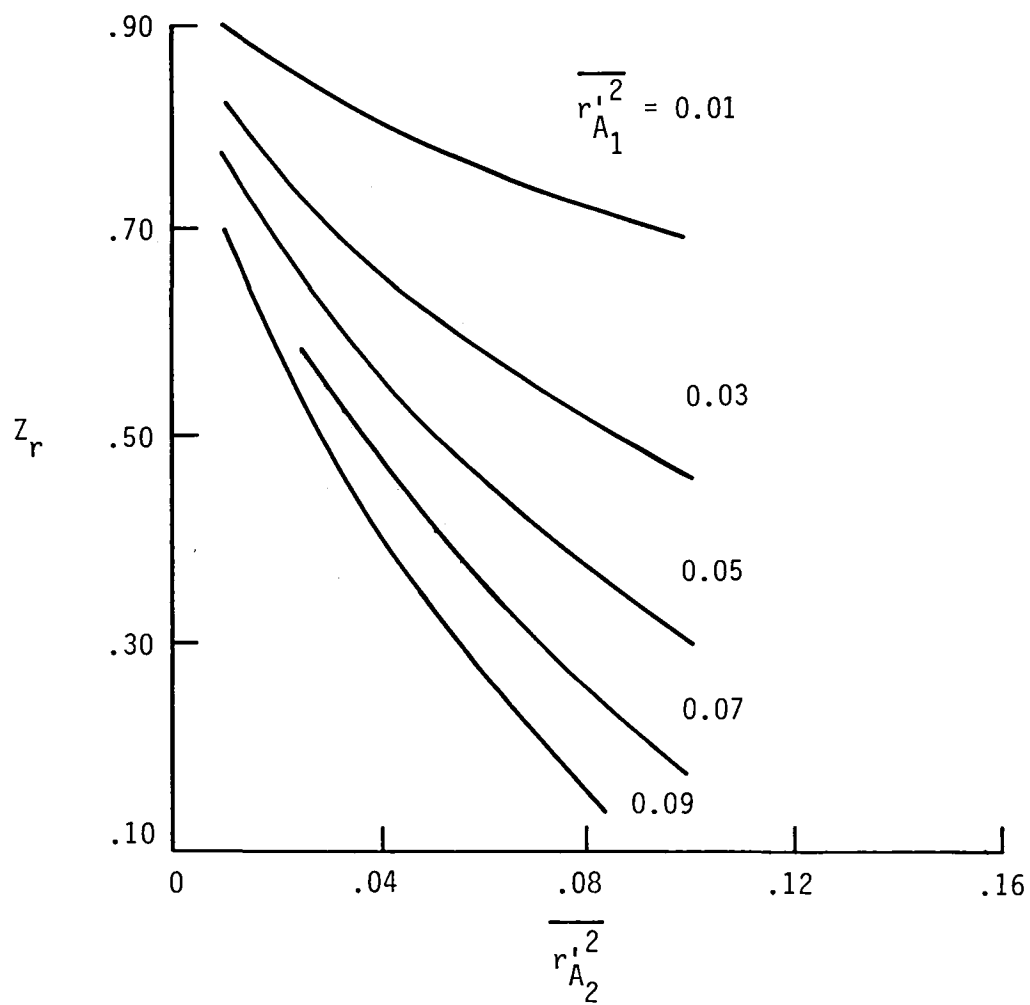
(a) $\bar{r}_{A_1} = 0.2$; $\bar{r}_{A_2} = 0.2$.

Figure 4.- Effect of species fluctuations on Z_r with $\rho^* = -0.9$.



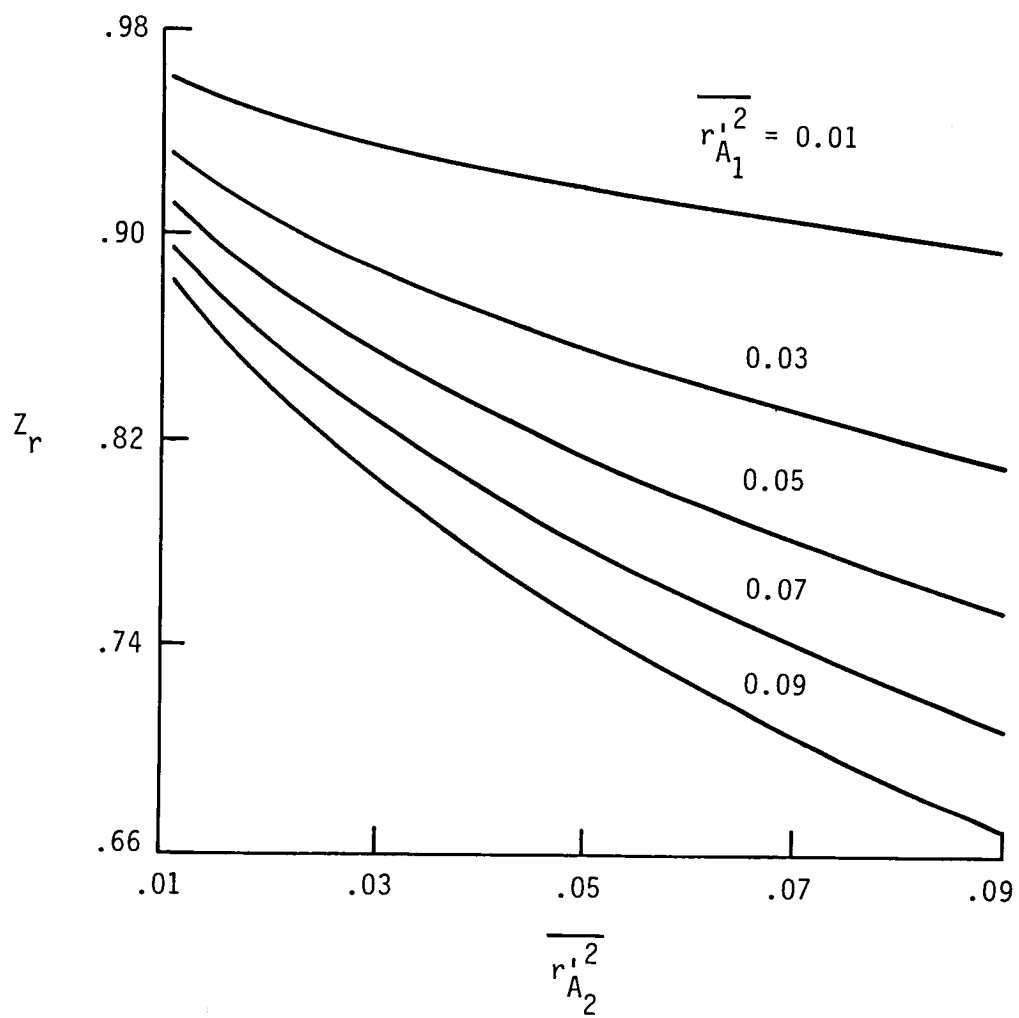
(b) $\bar{r}_{A_1} = 0.2$; $\bar{r}_{A_2} = 0.9$.

Figure 4.- Continued.



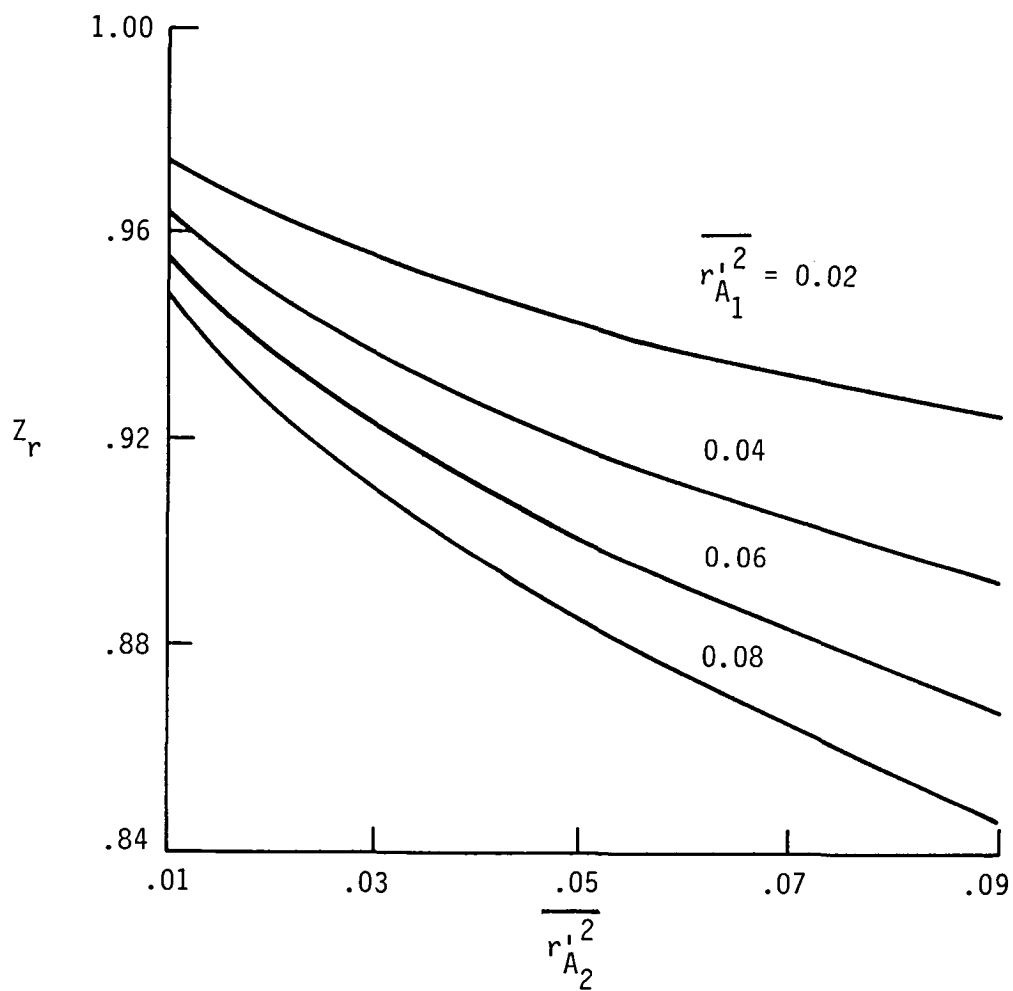
(c) $\bar{r}_{A_1} = 0.3$; $\bar{r}_{A_2} = 0.3$.

Figure 4.- Continued.



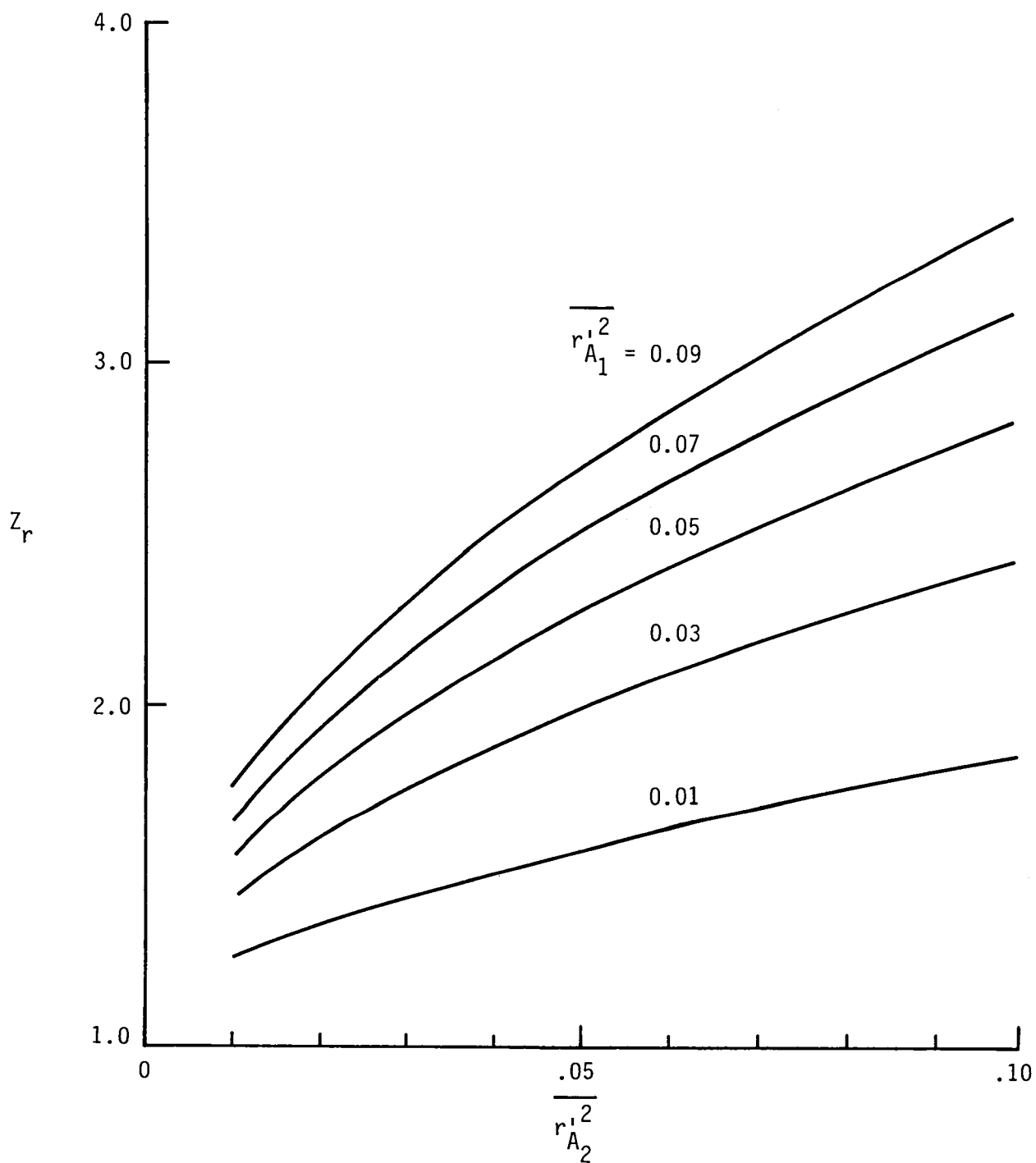
(d) $\bar{r}_{A_1} = 0.4$; $\bar{r}_{A_2} = 0.6$.

Figure 4.- Continued.



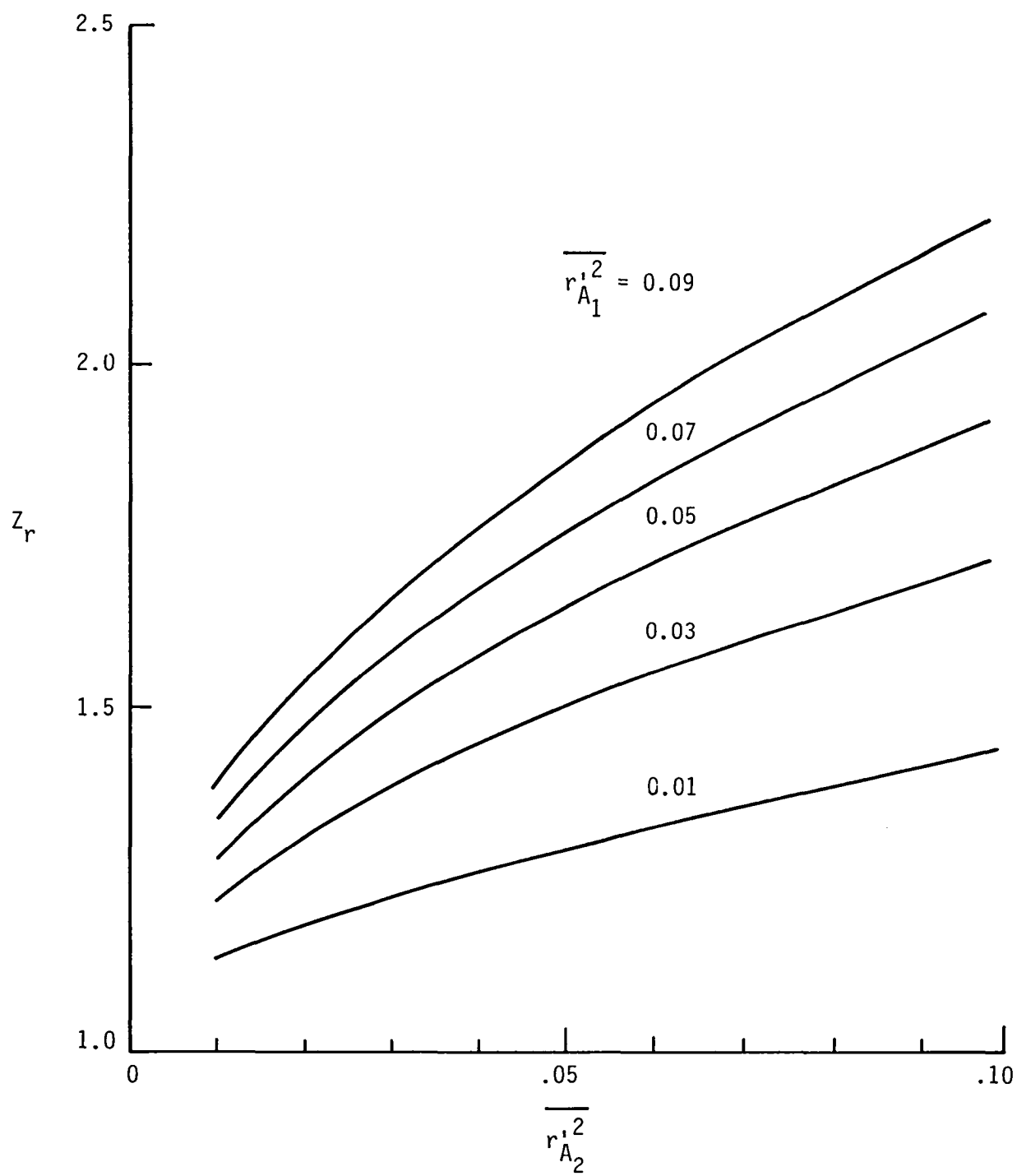
(e) $\overline{r_{A_1}} = 0.7$; $\overline{r_{A_2}} = 0.7$.

Figure 4.- Concluded.



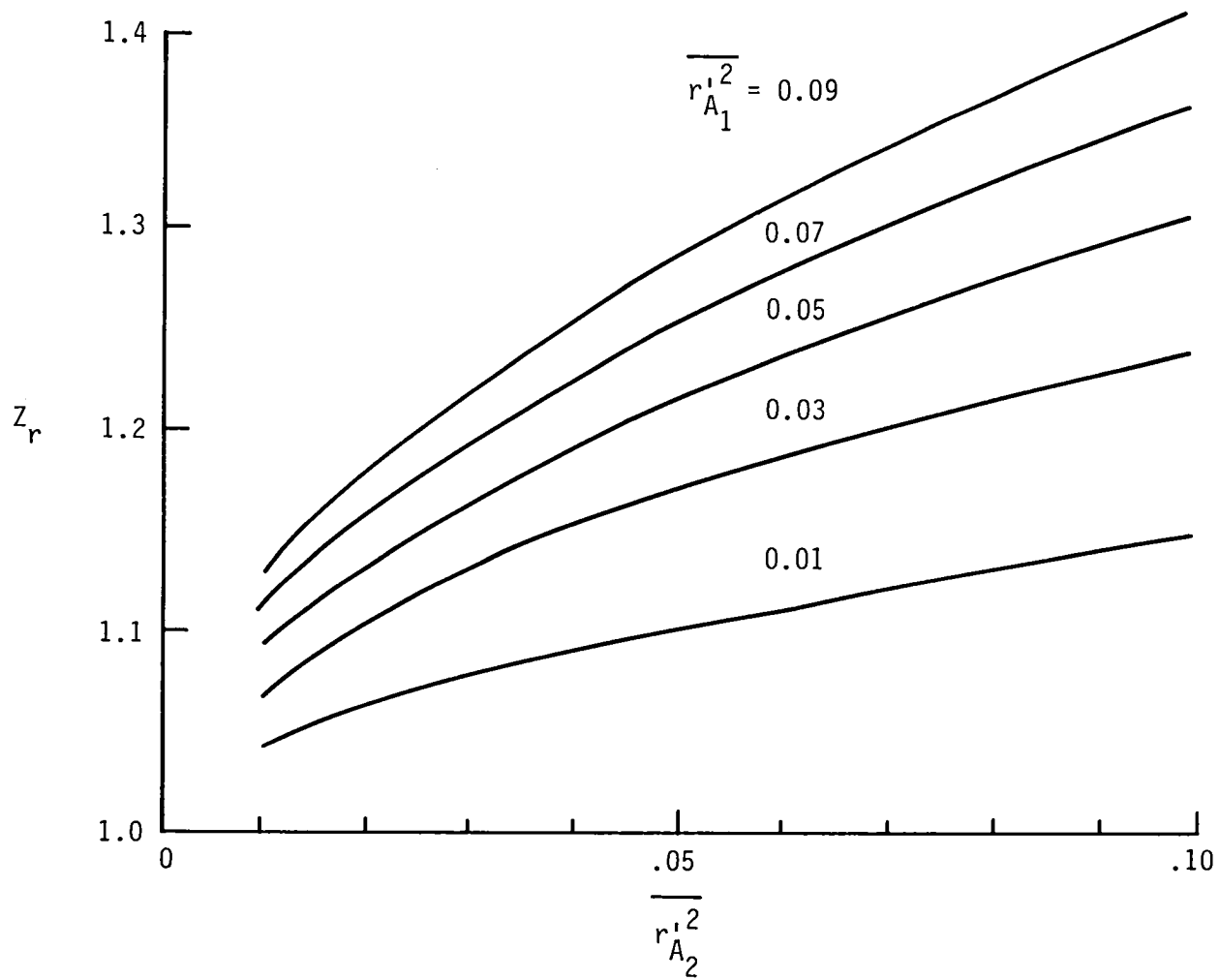
(a) $\overline{r_{A_1}} = 0.2$; $\overline{r_{A_2}} = 0.2$.

Figure 5.- Effect of species fluctuations on Z_r with $\rho^* = 0.9$.



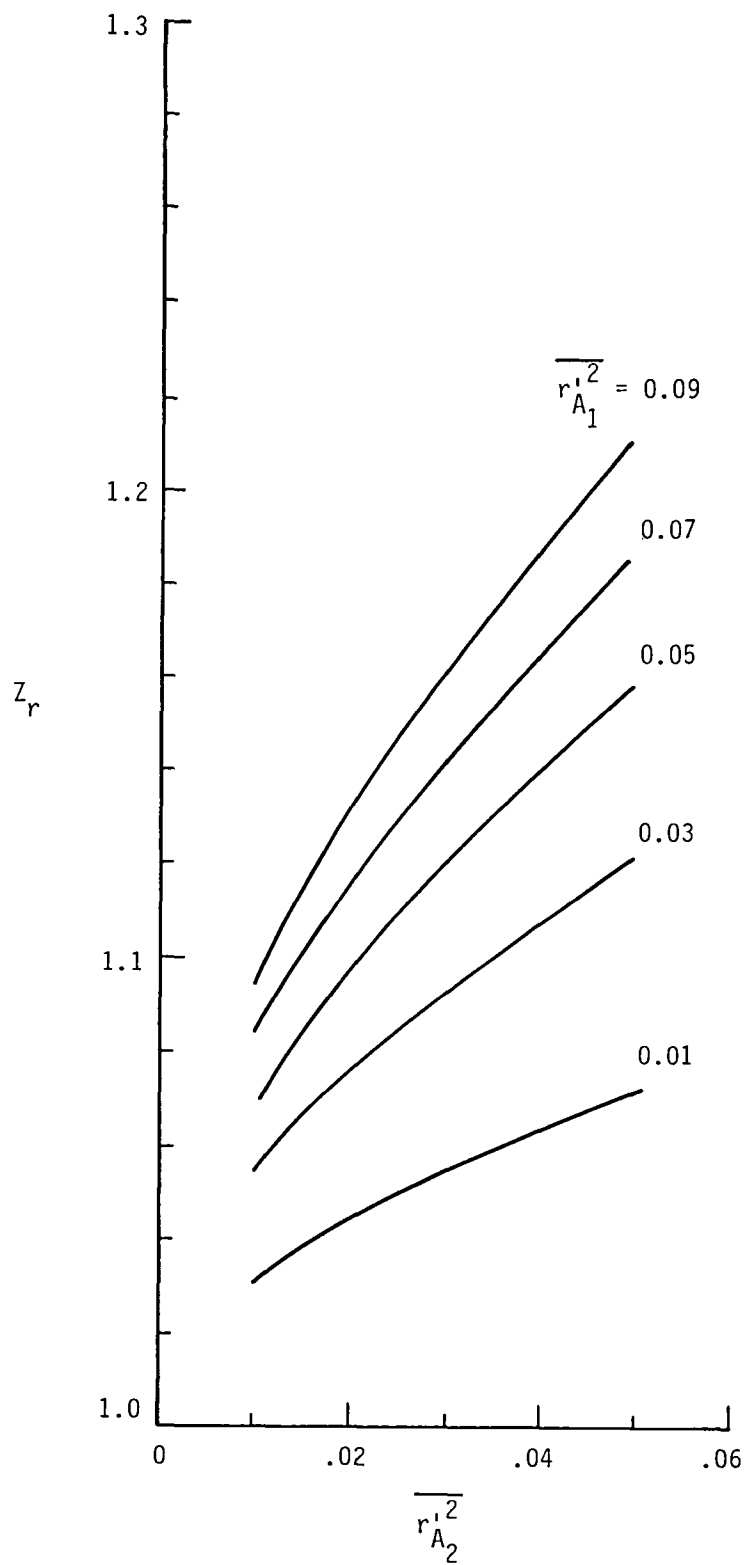
(b) $\overline{r_{A_1}} = 0.4$; $\overline{r_{A_2}} = 0.2$.

Figure 5.- Continued.



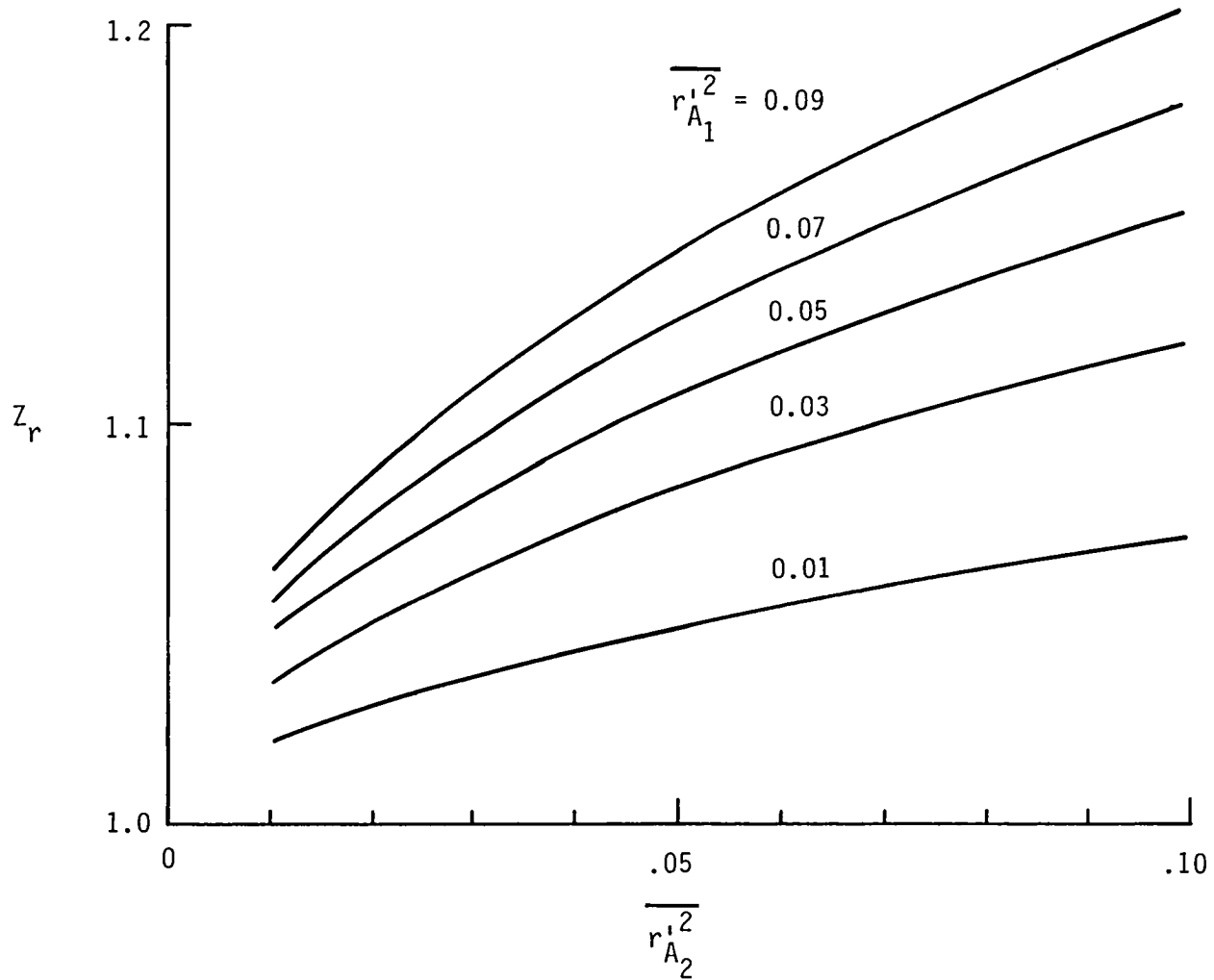
(c) $\overline{r_{A_1}} = 0.4$; $\overline{r_{A_2}} = 0.6$.

Figure 5.- Continued.



(d) $\bar{r}_{A_1} = 0.4$; $\bar{r}_{A_2} = 0.8$.

Figure 5.- Continued.



(e) $\bar{r}_{A_1} = 0.6$; $\bar{r}_{A_2} = 0.8$.

Figure 5.- Concluded.

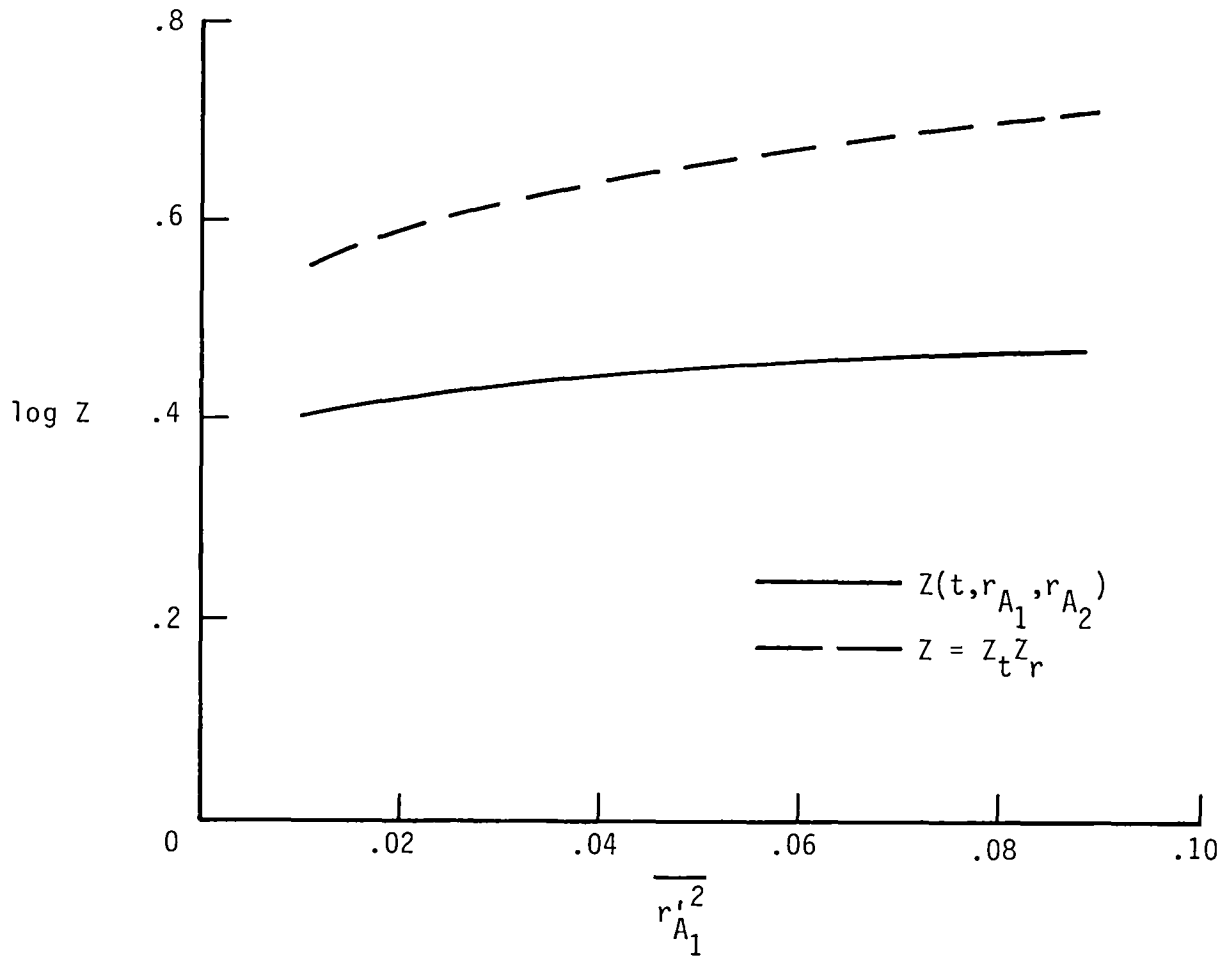
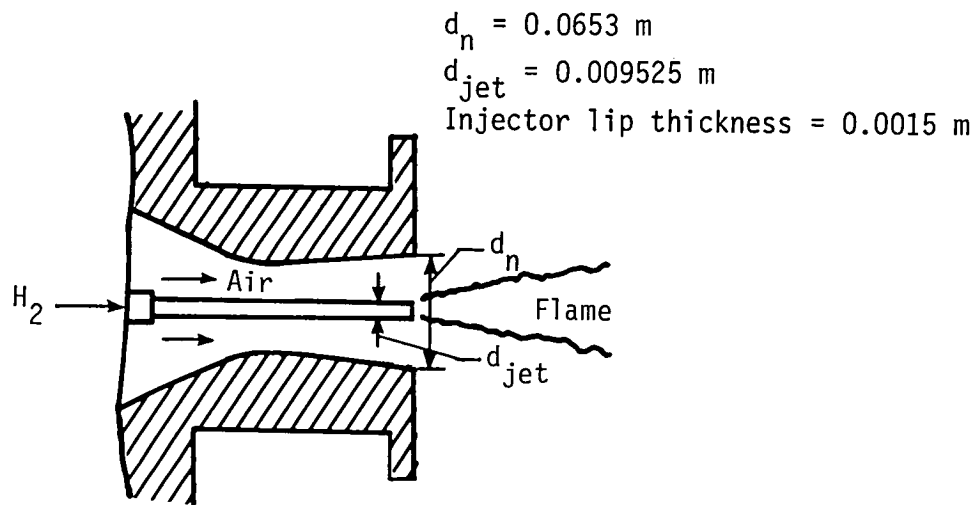


Figure 6.- Comparison of amplification ratios obtained from a three-variable pdf model and the proposed model. $\bar{t} = 0.4$; $\bar{r}_{A_1} = 0.4$; $\bar{r}_{A_2} = 0.5$; $\overline{t^{'2}} = 0.03$; $\overline{r_{A_2}^{'2}} = 0.03$; $\rho_{t-r_{A_1}}^* = -0.9$; $\rho_{t-r_{A_2}}^* = -0.9$; $\rho_{r_{A_1}-r_{A_2}}^* = 0.9$.



	Hydrogen jet	Free stream
Mach number	2.00	1.90
Temperature, K	251	1495
Velocity, m/s	2432	1510
Pressure, MPa	0.1	0.1
Mass fraction:		
a_{H_2}	1.000	0
a_{O_2}	0	0.241
a_{N_2}	0	0.478
a_{H_2O}	0	0.281

Figure 7.- Test-case flow parameters (ref. 25).

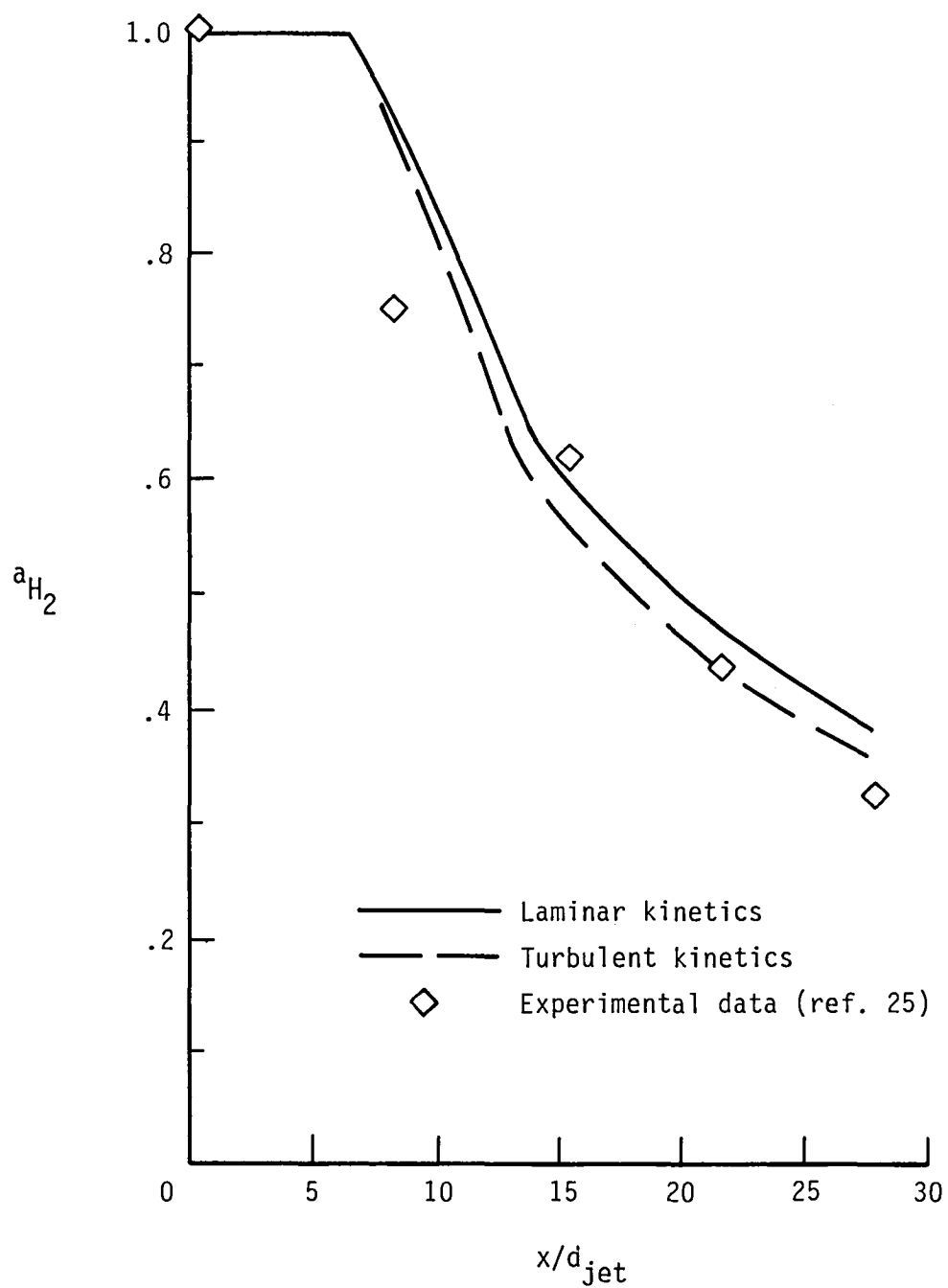
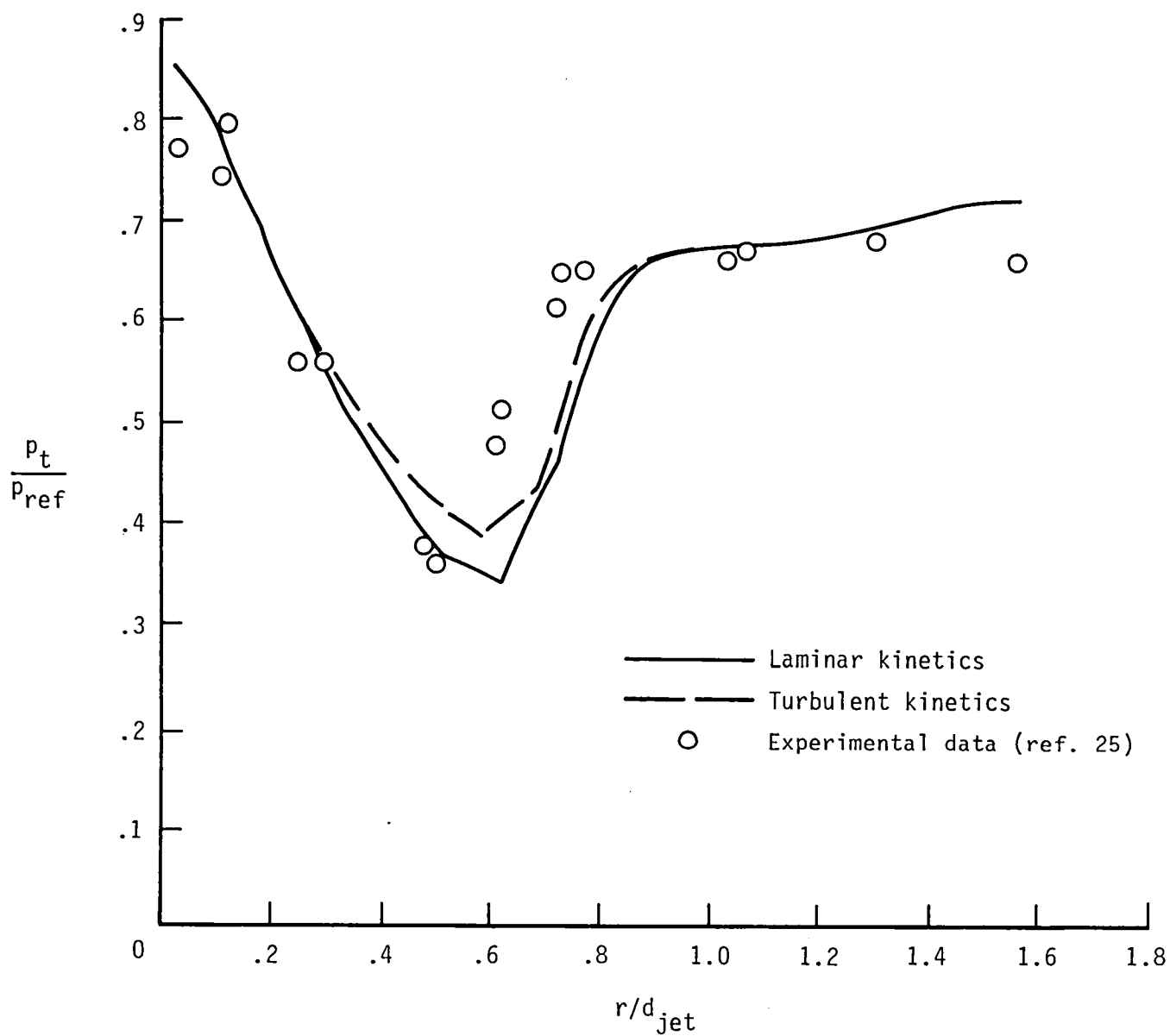
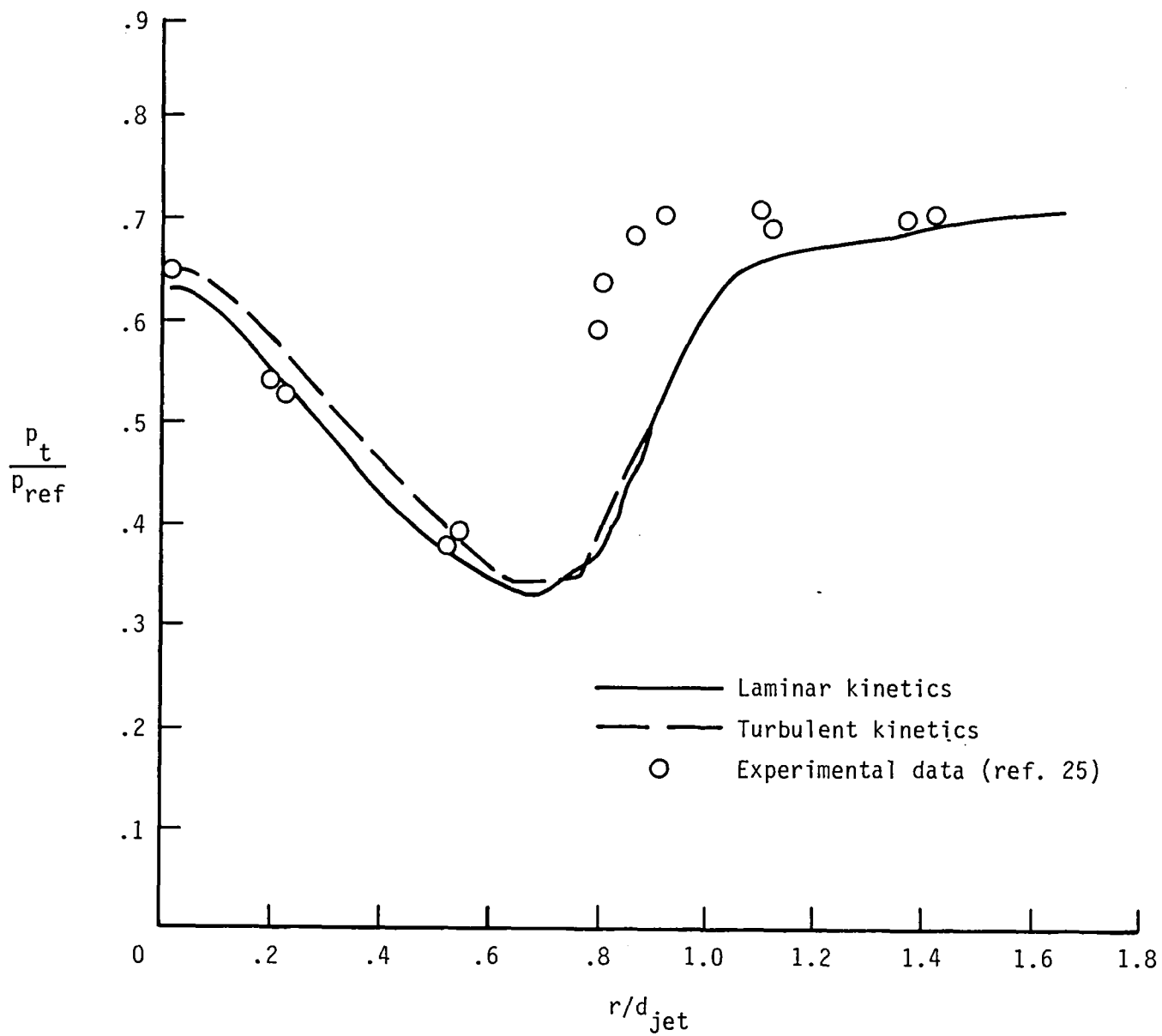


Figure 8.- Centerline mass fraction of hydrogen.



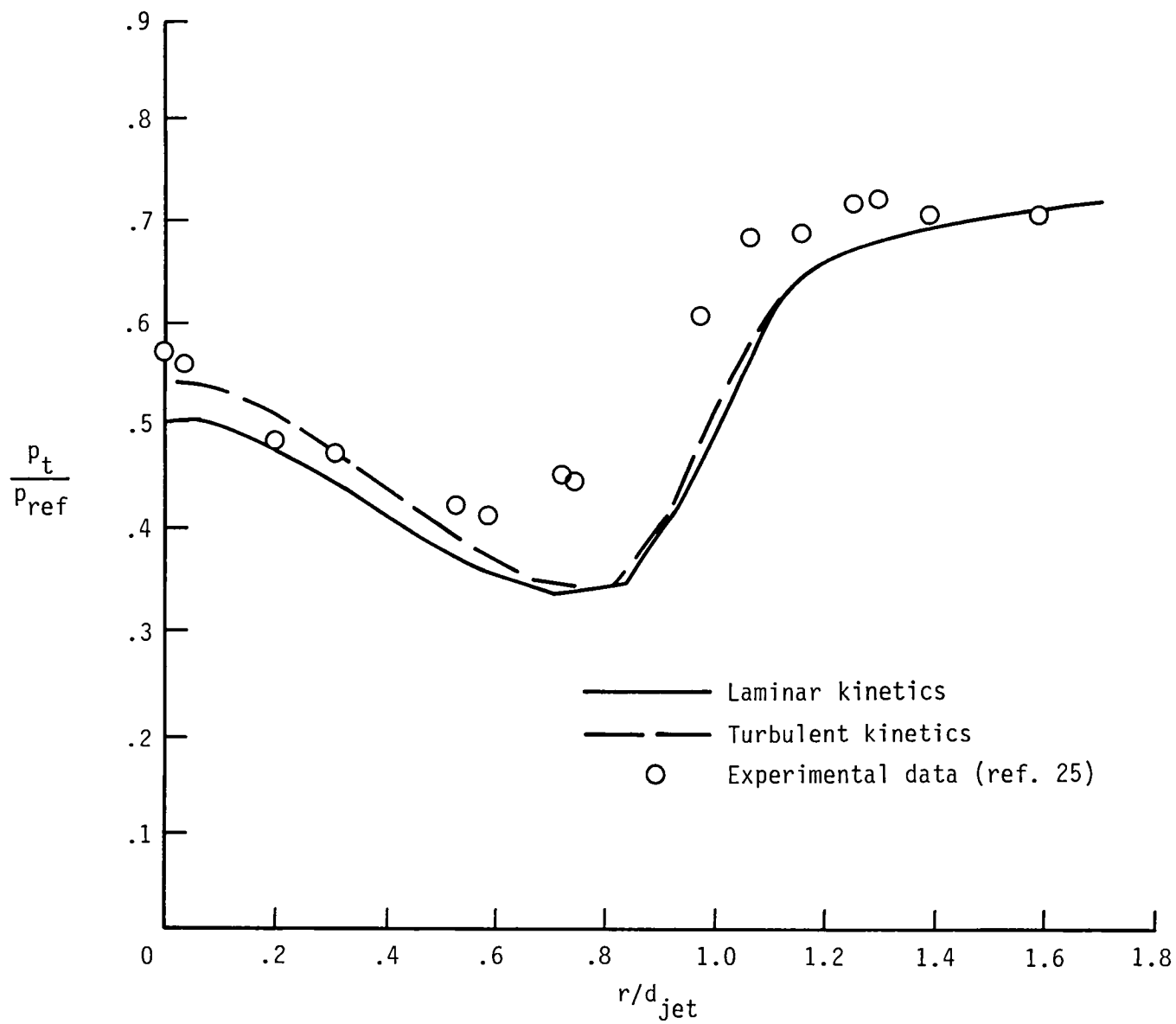
(a) $x/d_{jet} = 6.56$.

Figure 9.- Radial pitot-pressure profiles.



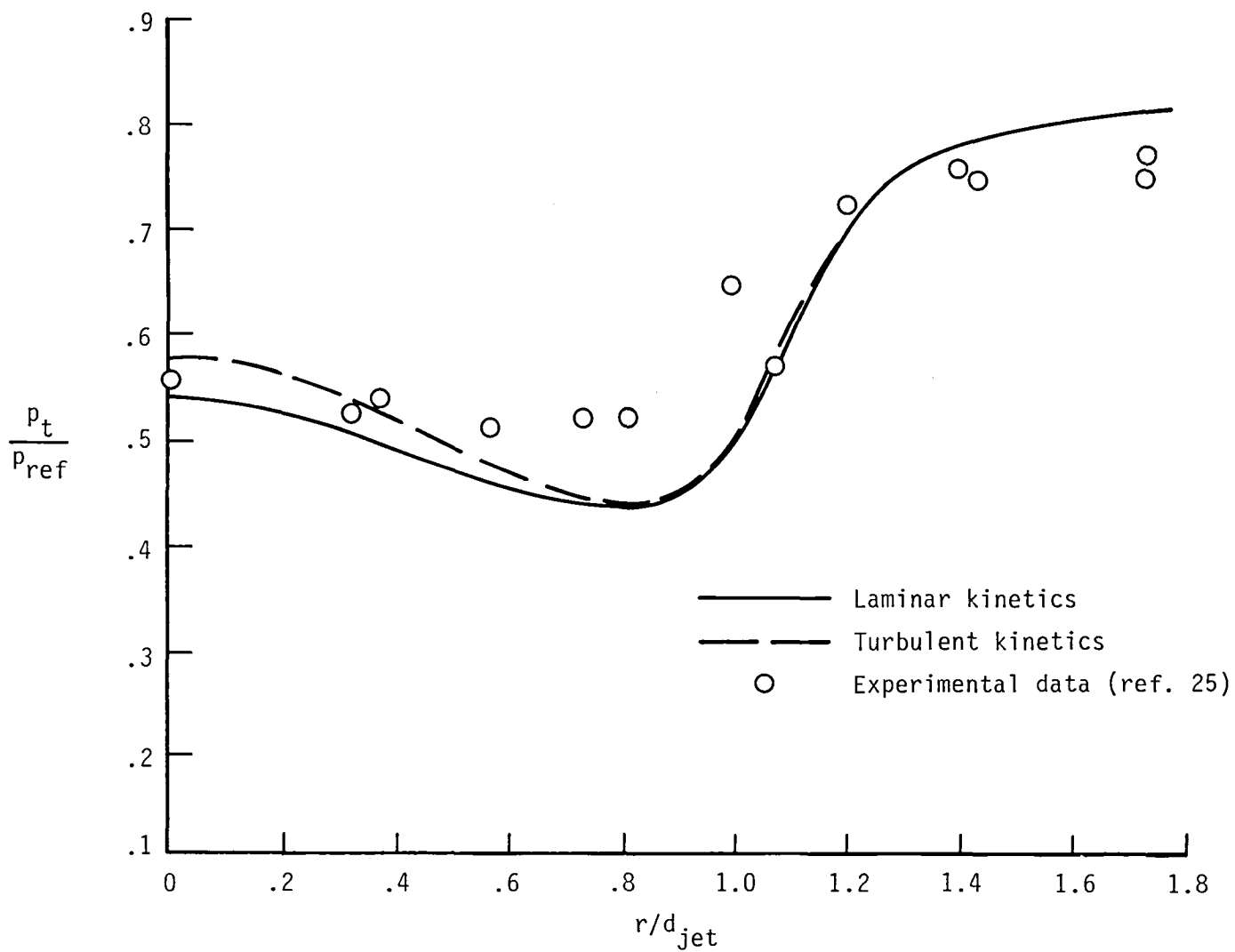
(b) $x/d_{jet} = 13.80$.

Figure 9.- Continued.



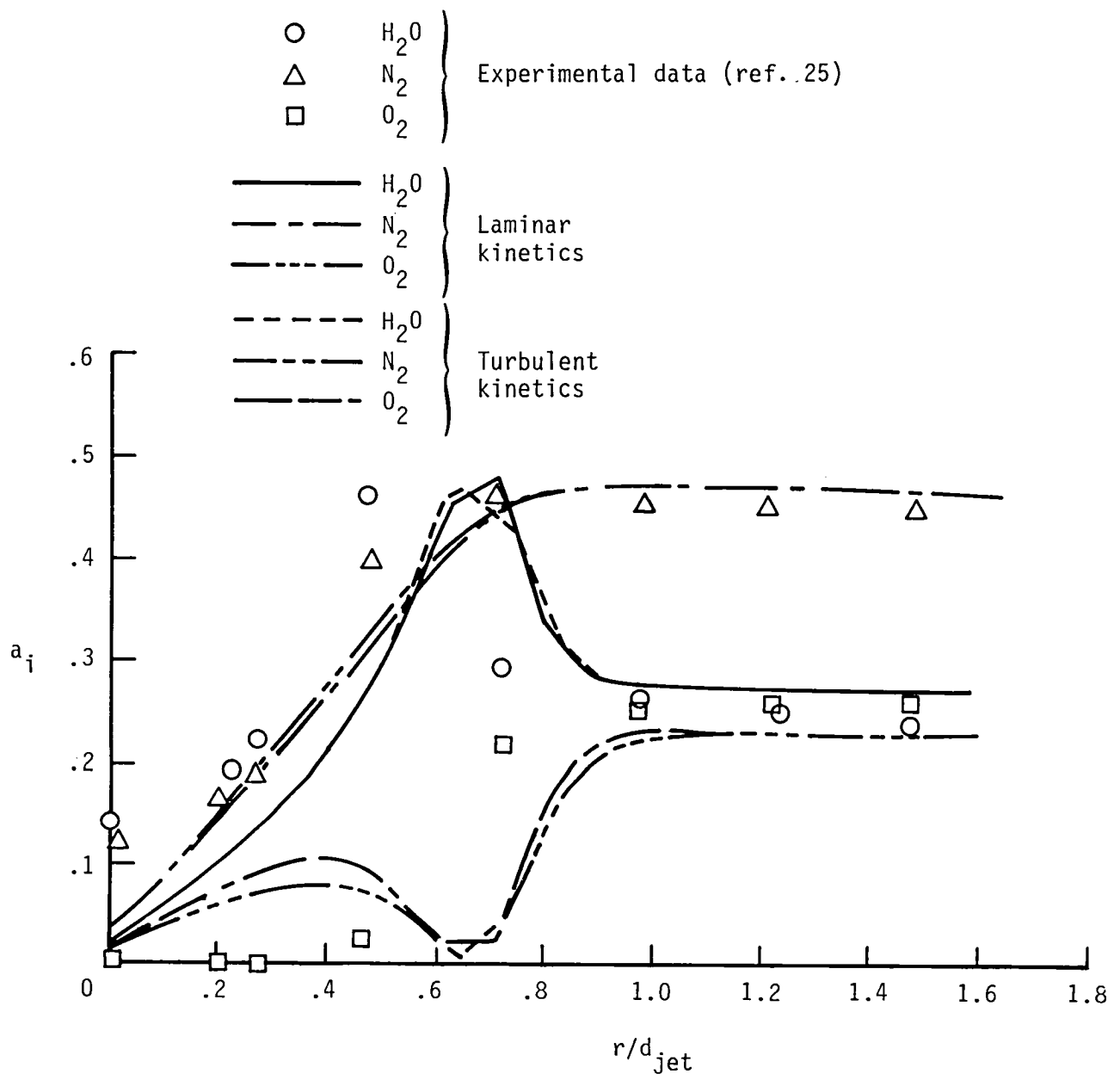
(c) $x/d_{jet} = 20.00$.

Figure 9.- Continued.



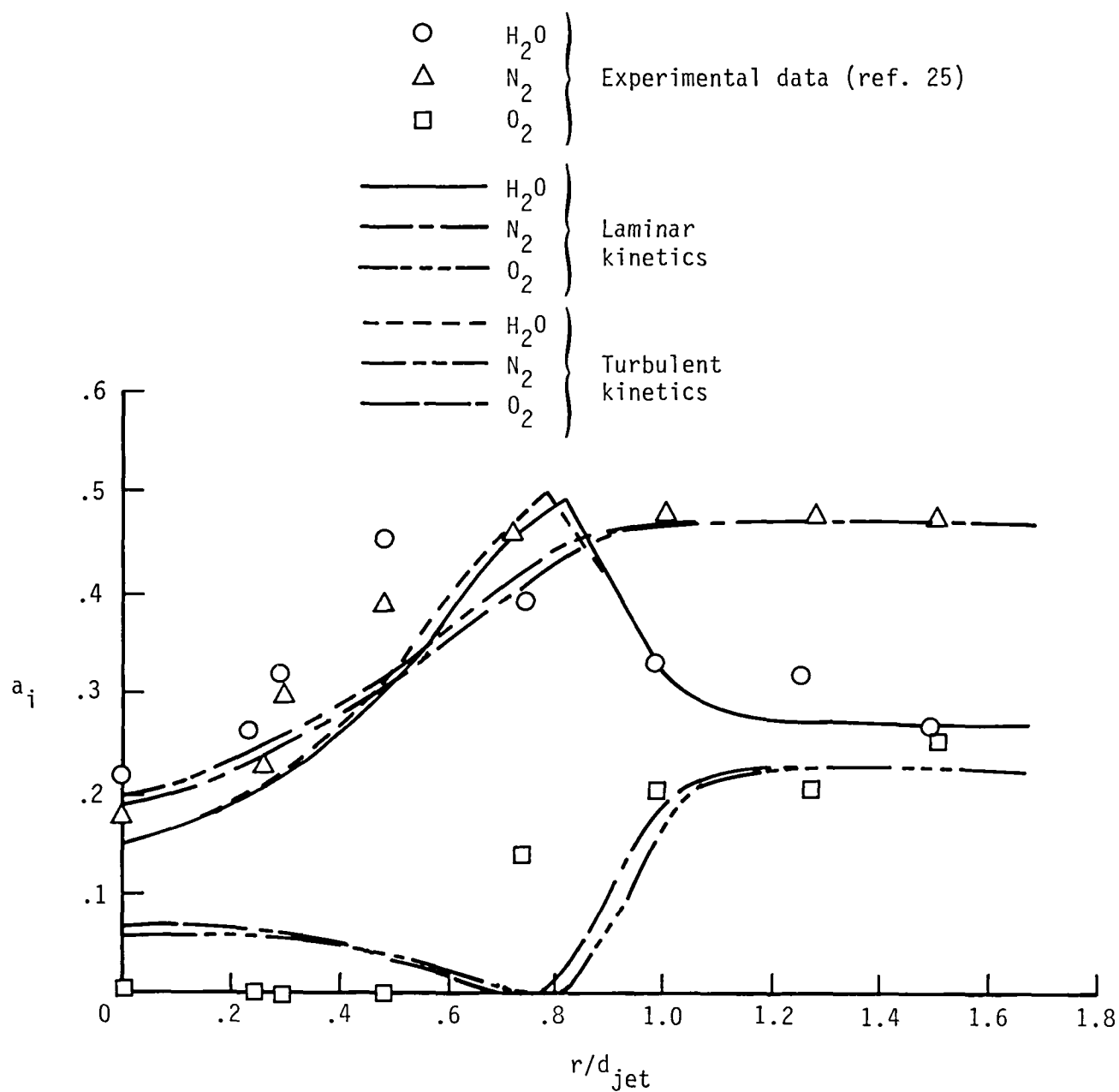
(d) $x/d_{jet} = 26.20$.

Figure 9.- Concluded.



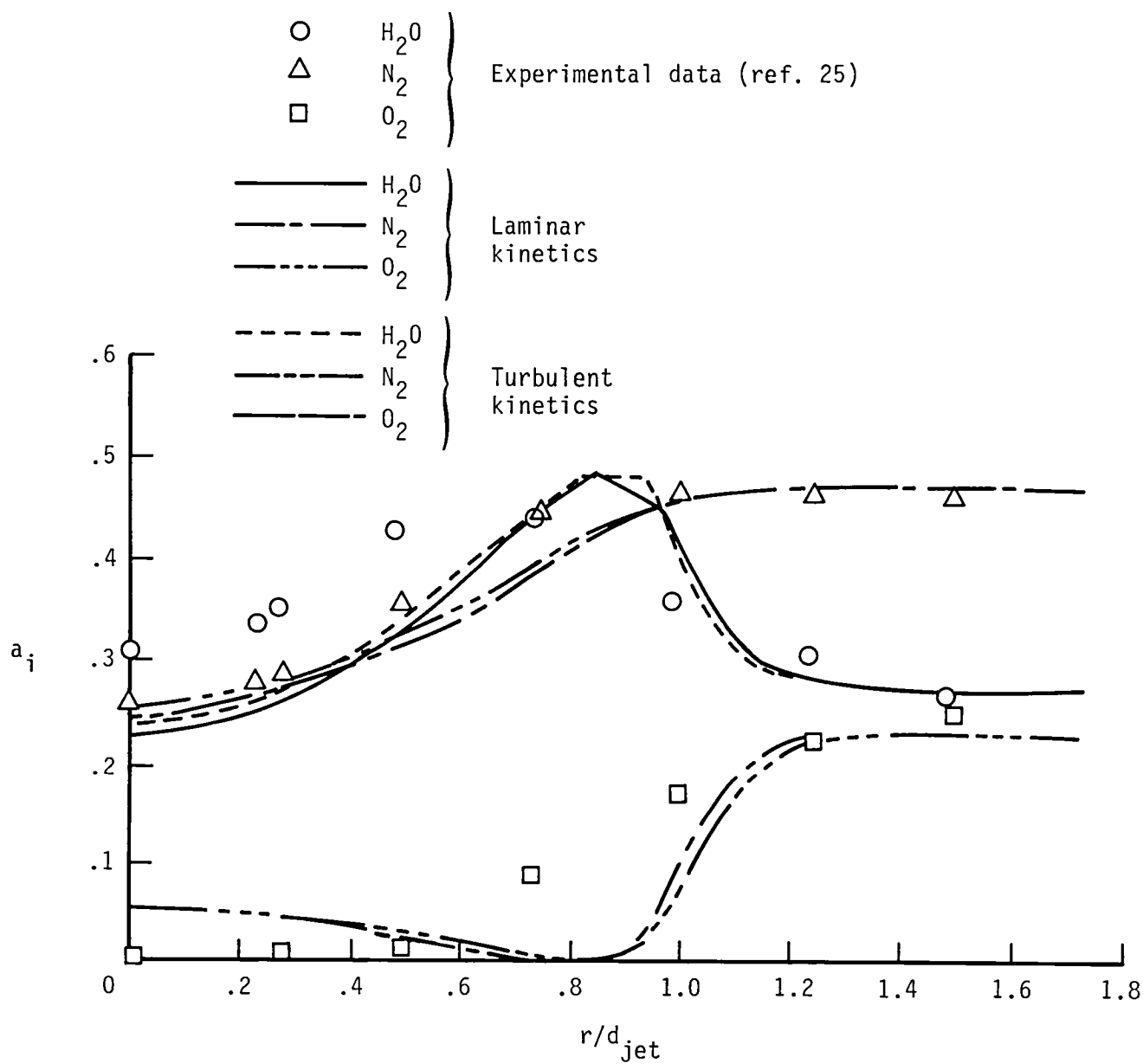
(a) $x/d_{jet} = 8.26$.

Figure 10.- Radial species-concentration profiles.



(b) $x/d_{\text{jet}} = 15.50$.

Figure 10.- Continued.



(c) $x/d_{\text{jet}} = 21.70$.

Figure 10.- Concluded.

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16. Abstract To account for the turbulent temperature and species-concentration fluctuations, a model is presented on the effects of chemical reaction rates in computer analyses of turbulent reacting flows. The model results in two parameters which multiply the terms in the reaction-rate equations. For these two parameters, graphs are presented as functions of the mean values and intensity of the turbulent fluctuations of the temperature and species concentrations. These graphs will facilitate incorporation of the model into existing computer programs which describe turbulent reacting flows. When the model was used in a two-dimensional parabolic-flow computer code to predict the behavior of an experimental, supersonic hydrogen jet burning in air, some improvement in agreement with the experimental data was obtained in the far field in the region near the jet centerline. Recommendations are included for further improvement of the model and for additional comparisons with experimental data.					
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